45th SACI
NATIONAL CONVENTION
CHEMISTRY: A WINDOW FOR CHANGE

WITS UNIVERSITY 100
1922
2022

ABSTRACT BOOK

SACI
South African Chemical Institute
Change through Chemistry

Table of Contents

Message from the SACI president

Dear SACI-45 delegates,

On behalf of the South African Chemical Institute, it is my great pleasure to welcome you to the 45th National Convention, taking place from 30 November to 5 December 2025 at the University of the Witwatersrand in Johannesburg. This gathering remains one of the most important events in our national chemistry calendar. It brings together scientists from academia, research institutions, and industry to explore, share, and advance the frontiers of chemical science.

This year's theme, "Chemistry: A Window for Change," captures the transformative spirit of our discipline. Chemistry continues to shape our world, from life-saving medicines and advanced materials to sustainable energy systems and environmental solutions. Through this lens of change, we will consider how our work can contribute to innovation, equity and a more sustainable future.

I am delighted that SACI-45 will once again serve as a platform for international engagement. We warmly welcome the leadership of our partner societies, including the International Union of Pure and Applied Chemistry, the Royal Society of Chemistry, the American Chemical Society and the Chemical Research Society of India. Your presence strengthens our shared commitment to advancing chemical sciences globally and deepens the collaborative bonds that enrich our community. We look forward to learning from your perspectives and exploring new partnership opportunities.

The scientific programme reflects the breadth and diversity of modern chemistry. The plenary and keynote speakers include world-class researchers, thought leaders and innovators. I am particularly excited about the special quantum science session, aligned with the International Year of Quantum Science and Technology, which will showcase emerging quantum approaches and their impact on chemical research.

The University of the Witwatersrand provides an inspiring setting for SACI-45, blending historic character with state-of-the-art scientific and immersive facilities. We hope you will enjoy the atmosphere of this dynamic campus and the vibrant environment it offers throughout the event.

This Convention is not only about scientific exchange but also about people. It is about the relationships we build, the collaborations we initiate and the mentoring that supports researchers at every stage of their careers. Whether you are a senior scientist or a postgraduate student presenting your first abstract, I encourage you to engage fully, ask bold questions and take every opportunity to connect.

I extend my sincere thanks to the Local Organising Committee at Wits, led by Dr Manoko Maubane-Nkadimeng and Prof. Caren Billing, for their dedication and hard work in bringing SACI-45 to life. I also thank our sponsors for their generous support, which enables us to host a high-quality convention that benefits the entire chemistry community. And to each of you, our delegates, thank you for contributing your expertise, your enthusiasm and your commitment to SACI 45.

I wish you a memorable, stimulating and rewarding week. Enjoy the scientific programme, the networking opportunities and the vibrant city of Johannesburg. Together, let us harness the power of chemistry to inspire meaningful change.

Warm regards
Nikoletta B. Bathori

CPD Credits: 5

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Message from the chairs of the organising committee

Dear SACI-45 Delegate

Warm welcome to the University of the Witwatersrand in the city of gold, Johannesburg, and thank you for being part of the 45th National SACI Convention. We hope that you will have an enjoyable and productive meeting, attending the various sessions in the scientific programme as well as the range of special sessions that have been organised. This includes celebrating the International Year of Quantum Science and Technology and hosting an entrepreneurship event. Together, we look forward to fostering growth and collaboration that will strengthen our scientific community and inspire future innovation.

Of course, it is not all work. We have prepared a vibrant social programme that offers opportunities to connect, build relationships, and ensure that the benefits of this meeting extend well beyond the event itself. We also invite you to connect with our exhibitors and explore the posters on display in the exhibition hall.

We would like to extend our sincere gratitude to the Local Organising Committee for their tireless work behind the scenes, and to our sponsors and partners for their invaluable support. Most importantly, we thank all of you, our participants, for contributing your time, energy, and expertise to SACI-45.

Wishing you all the best
Caren Billing and Manoko Maubane-Nkadimeng

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Conference Chair


Dr Manoko Maubane-Nkadimeng (WITS)
Co-Chair


Prof. Neil Coville (WITS)
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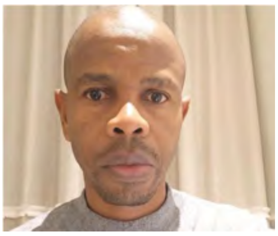
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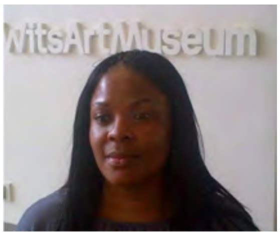

Ms. Kelebogile Tadi (WITS Event Office)
Event Co-ordinator

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Previous SACI Conventions

No.	**Host Section**	**Date**	**City**	**Chair**
44	Western Cape	8 – 13 Jan 2023	Stellenbosch	Prof Catharine Esterhuysen
43	Northern Gauteng	3 - 7 Dec 2018	Pretoria	Dr Richard Mampa
42	KwaZulu-Natal	29 Nov - 4 Dec 2015	Durban	Prof Bice Martincigh
41	Eastern Cape	1 - 6 Dec 2013	East London	Prof Adebola Oyedeji
40	Gauteng	16 - 21 Jan 2011	Johannesburg	Prof James Darkwa
39	Western Cape	30 Nov - 5 Dec 2008	Stellenbosch	Prof Len Barbour
38	KwaZulu-Natal	3 - 8 Dec 2006	Durban	Prof Sreekanth Jonnalagadda
37	Northern Gauteng	4 - 9 July 2004	Pretoria	Prof Jan Boeyens
36	Eastern Cape	30 June - 5 July 2002	Port Elizabeth	Dr Chris Woolard
37	Transvaal	24 - 29 Sept 2000	Potchefstroom	Prof Ernst Breet
38	Natal	6 - 10 July 1998	Durban	Prof Trevor Letcher
33	Western Cape	29 Jan - 2 Feb 1996	Cape Town	Prof James Bull
32	Northern Transvaal	30 Jan - 3 Feb 1994	Halfway House	Dr Willie van Niekerk
31	Eastern Cape	24 - 27 July 1991	Grahamstown	Prof Trevor Letcher
30	Western Province	15 - 20 Jan 1989	Cape Town	Dr GML Cragg
29	Natal	6 - 10 July 1987	Durban	Prof Mike Laing
28	Western Province	30 Jan - 3 Feb 1984	Stellenbosch	Prof Ivan Green
27	Pretoria Section	25 July - 1 Aug 1980	Pretoria	Dr Jan Boeyens
26	Eastern Cape	1979 for 3.5 days	Port Elizabeth	Prof Andre Goosen
25	Northern Transvaal	31 Jan - 4 Feb 1977	Johannesburg	Dr VM Lovell
24	Natal	14 - 18 July 1975	Durban	Dr Terence MS Higgins
23	Western Province	28 Jan - 1 Feb 1974	Cape Town	Dr GML Cragg
22	Northern Transvaal	3 - 7 July 1972	Pretoria	Dr A Jordaan
21	Eastern Province	1 - 4 Feb 1971	Grahamstown	Dr DEA Rivett
20	Natal	10 - 14 July 1967	Durban	Mr MP Theunissen
19	Western Province	Feb-66	Stellenbosch	Dr M Lamchen
18	Northern Transvaal	Jul-64	Pretoria	Dr TL Webb
17	Eastern Province	15-19 July 1963	Port Elizabeth	Mr JM Tucker
16	Natal	Jul-62	Pietermaritzburg	Prof Israelstam
15	Natal	17 - 21 July 1961	Durban	Mr JL du Toit
14	Western Province	8 - 12 Feb 1960	Cape Town	Prof LH Ahrens

No.	Host Section	Date	City	Chair
13	Northern Transvaal	20 - 24 July 1959	Pretoria	Mr CC van der Merwe
12	Eastern Province	14 - 18 July 1958	Port Elizabeth	VA Morris
11	Natal	8 - 12 July 1957	Durban/ Pietermaritzburg	Mr JE Worsdale
10	Transvaal	24 - 29 Sept 1956	Johannesburg	Dr SS Israelstam
9	Western Cape	6 -10 Feb 1955	Cape Town	Dr Lamchen
8	Northern Transvaal	30 Aug - 4 Sept 1954	Pretoria	Dr AJ Petrick
7	Natal	6 - 10 July 1953	Durban	Dr GC Scully
6	Transvaal	30 June - 4 July 1952	Johannesburg	Dr SS Israelstam
5	Eastern Cape	1 - 6 October 1951	Port Elizabeth	Mr L-F Addis-Smith
4	Western Cape	Sep-50	Cape Town	Mr AL Abbott
3	Natal	20 - 23 July 1949	Durban	Mr A Gregory
2	Northern Transvaal	June 1948 (4 days)	Pretoria	Dr ER Orchard
1	Transvaal	27 - 29 June 1947	Johannesburg	Mr CF Lindemann

General Information

Weather in Johannesburg

The weather in Johannesburg is predicted to be cool (between 12°C and 25°C) and rainy, so please bring an **umbrella** and something warm to put on.

Transport From OR Tambo Airport to the University of the Witwatersrand

- Gautrain from OR Tambo: https://www.gautrain.co.za/. Only use Rosebank Station, then road transport as required as below.
- EZ Shuttle: https://www.ezshuttle.co.za/
- E-hailing services e.g. Uber, Bolt.

Access to the University

- All delegates who enter campus must have a valid ID or Passport or Driver's License.
- ***Sunday***:
  Arriving by car – use the north or south entrances on Yale Road. Parking as demarcated on the map.
  Pedestrian access – only at Sutton Place, from Jorrisen Street at the intersection with Eendracht Street.
- ***Monday – Friday***:
  Arriving by car and pedestrian access – use the Enoch Sontonga entrance.

Contact Details During Conference

General enquiries: 061 282-3477
Emergency contact: 24-hour Security at the Great Hall Foyer, East Campus (011) 717-4444 and West Campus (011) 717-6666.
ER24 ambulance: 084 124

Safety

The campus is a secure and safe venue for the Convention. But as is normal, please take care of your personal belongings on campus and don't leave bags, computers etc. unattended. When off campus, ensure that your car doors are locked and windows are closed

Sunday, 30 November: *East Campus*

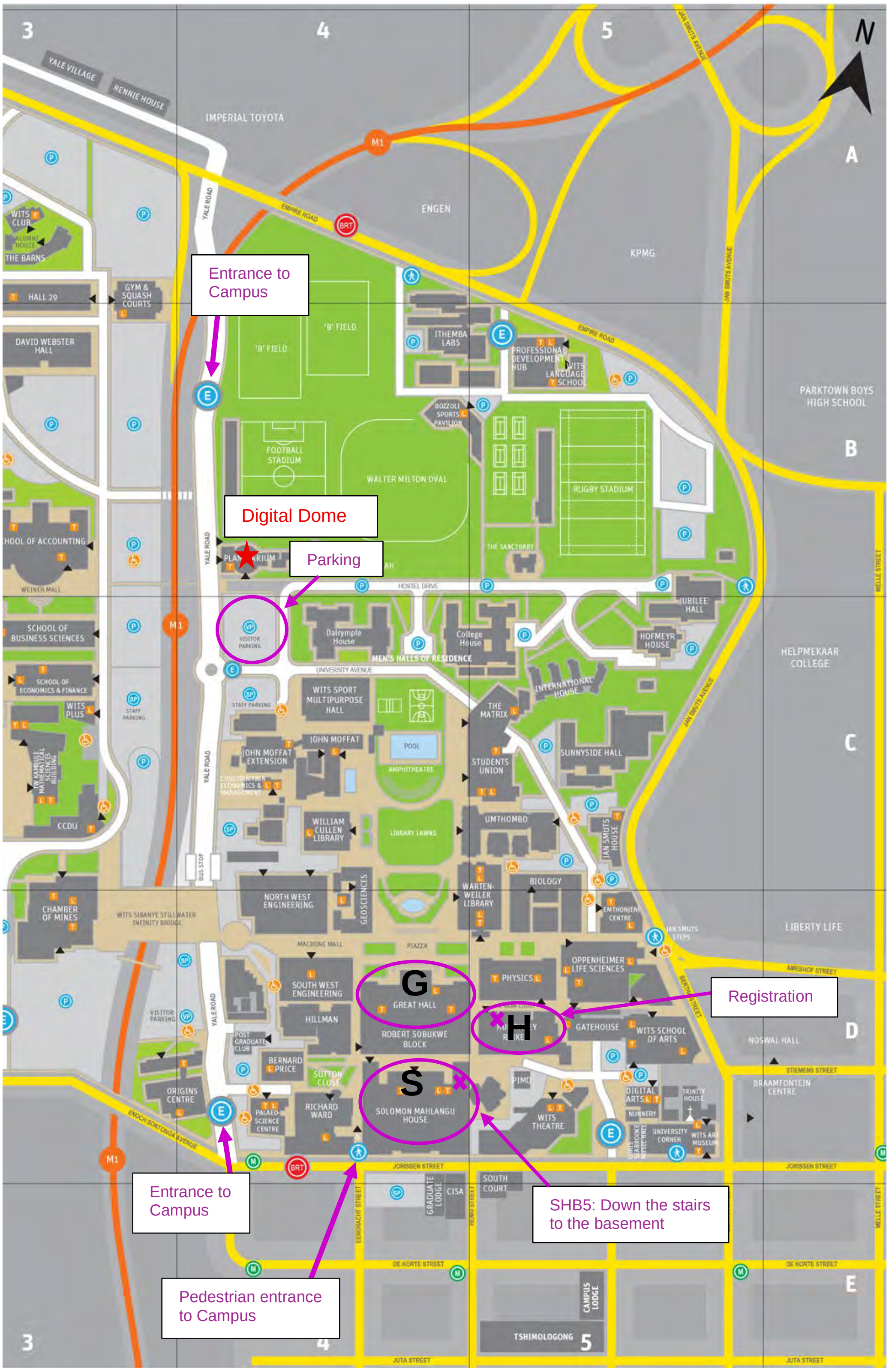
H – Registration: Humprey Raikes (Chemistry) Building

S –Solomon Mahlangu (old Senate House):

Entrepreneurship event: SHB5

Ice breaker: Solomon Mahlangu Concourse

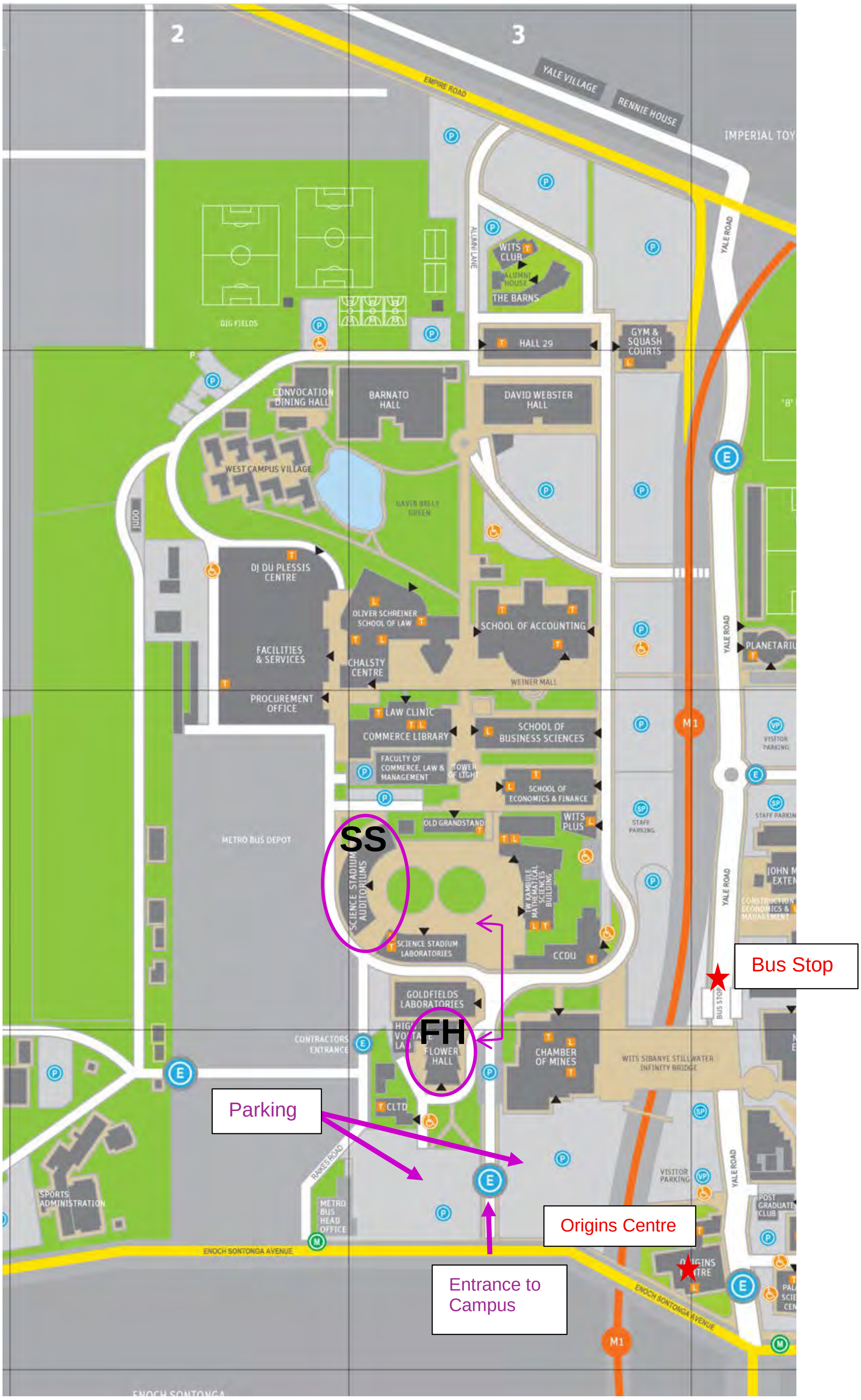
G – Opening ceremony: Great Hall



Monday – Friday, 1-5 December: *West Campus*

SS – Lecture theatres: Wits Science Stadium, WSS 2-5

FH – Exhibitions and Posters: Flower Hall, ground and 1st floor



Registration

Registration will take place at the Humprey Raikes (Chemistry) Building, East Campus, from 12:00-18:30 on Sunday 30 November. From Monday to Thursday 1-4 December, registration will take place at the Science Stadium, West Campus.

Name Tags

Please wear your name tags at all times to gain access to the university and during the convention proceedings. Vouchers for drinks are included with your name tags as per your registration.

Internet Facilities

You can connect to the Wits-Guest wi-fi using: **Username** 670b7 **Password** 7W47hea; (including the semicolon). Alternately, *eduroam* access is available.

Lecture venues

All oral presentation will take place at the Sciences Stadium, where the lecture venues are adjacent to each other allowing easy movement between parallel sessions.

Speaker Information

Slides should be prepared in MS PowerPoint using either 16:9 (wide screen) or 4:3 (standard) slide size. Slides should preferable be emailed to AV support at colinvw@lantic.net or loaded in the venue using a USB flash drive for large files. This must be done latest before the plenary session for the morning slots and at the start of lunch for all the afternoon slots. **Please save your file using the following format to avoid confusion: Surname_Day_PresentationNo** (e.g., Smith_Mon_O190.pptx). Use of your own computer is not possible. A timer will be provided in the lecture venue, please ensure time is strictly adhered to (**includes** 5 minute Q&A).

Poster Presenter Information

Posters should be prepared in A0 size portrait orientation. Poster sessions will be held in the Flower Hall on Monday 1 December and Tuesday 2 December. *Please consult the abstract book to identify your poster number*. **All** posters need to be put up by **Monday lunchtime**. Materials to hang your poster will be provided. If you have an **odd-numbered** poster, please be present at your poster on **Monday** evening and if you have an **even-numbered poster** please be present at your poster on **Tuesday** evening. Posters should be taken down by lunchtime on Friday.

Refreshments

Morning and afternoon tea and coffee will be served in the exhibition area in the Flower Hall on both the ground and first floors according to the programme. Water coolers will be available to fill provided water bottles. Drink vouchers are provided for the various functions (no additional water will be provided).

Lunches

Bagged lunches will be provided daily at the Science Stadium which can be eaten in the area in the Science Stadium and the Old Grandstand. The second floor of the Flower Hall will also be available in case of rain. Please use the provided dustbins for rubbish.

Shops and Banking Facilities

Additional venues offering food and beverages on West Campus include:
- **VidaE Café** on the Amic Deck.
- **Maphelo @ Tower of Light**
- **Zesti Lemonz**
- **FoodArt@Origins centre**
- **Wits Club** run by Olives and Plates

The Matrix Student Centre on East Campus is a vibrant student hub that includes food stores, books, computer shops, printing and stationery outlets, banks and ATMs.

Conference Photograph

A conference group photograph will be taken on Monday, 1 December, at 12h40 (before lunch) on the stairs next to the Old Grandstand, weather permitting.

Baggage Area

A secure baggage storage area will be provided on Friday in the laboratories to facilitate departures.

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Bruno Steiner Lab Consultancy is a level 2 BBBEE Contributor

Social Programme

Ice breaker (Sunday 30 November, 18:30-20:30): The cocktail function will take place in the Solomon Mahlangu concourse. Dress code is casual.

Braai at Sci-Bono Discovery Centre (Monday 1 December, 18:00-22:00): Sci-Bono is a world-class science centre that supports maths, science and technology education and offers innovative, dynamic learning experiences that contribute to building South Africa's science, engineering and technology capacity. Buses will take us to Sci-Bono in Newtown where we can peruse the centre and enjoy a braai (barbeque) together. All buses leave from the bus stop in Yale Road. Dress code is casual.

Periodic Pursuit (Tuesday 18h00-22h30): For those who opted to take part in the team building event, get ready for a high-energy, brain-teasing journey where science meets strategy! Periodic Pursuit is not your ordinary challenge, it is a quest against time and intellect, where every clue unlocks a new path on your blueprint of scientific discovery. Afterwards supper will be served at the Science Stadium, followed by some fun filled Karaoke in the Flower Hall, 2nd floor.

Excursions (Wednesday 13h30): A range of excursions were offered. The sticker on your name badge will remind you of which one you opted for, if any.
Lion and Rhino Nature Reserve: Grab your lunch and head to the bus stop in Yale Road. Buses depart at 13:30 and will return at about 17:30.
Apartheid Museum: Grab your lunch and head to the bus stop in Yale Road. The bus departs at 13:30 and will return at about 16:30.
Digital Dome (East Campus): The show runs from 14:00 – 15:00. Please make sure you are there 15 minutes before to be seated.
Origins Centre (West Campus): The tour starts at 14:00 runs for 90 minutes. Please make sure you are there 10 minutes before.

Gala Dinner (Thursday 18:00): The dinner with be held at Thaba Eco, nestled in the Klipriviersberg Nature Reserve area, providing stunning views of nature in the heart of Johannesburg. Buses will depart from the bus stop in Yale Road at 18:00 and start returning in intervals from 22:00 until 23:30 (buses will leave once full). We are looking forward to an evening of good food and dancing. Dress code is smart casual.

Programme

30 November 2025 - Sunday	
12h00-18h00	Registration Venue: Foyer Humphrey Raikes Building
14h00-16h00	Entrepreneurship Event **O6 - David Fine - Everyone can innovate** Panel Discussion chaired by Sabelo Venue : SHB5 Chair: Alexandra Flusk
16h00-16h15	Move to opening ceremony at the Great Hall
16h15-17h00	**Opening Ceremony** LOC: Manoko Maubane-Nkadimeng (10 min) WITS VC: Zeblon Vilakazi (10 min) IUPAC President: Ehud Keinan (5 min) RSC President: Robert Mokaya (5 min) CRSI Vice-President: Narayanaswamy Jayaraman (5 min) SACI President: Nikoletta Bathori (5 min) Chair: Caren Billing
17h00-17h50	**O18 - SACI Gold Medal 2023: Roger Hunter** Organic synthesis in South Africa: For business or pleasure?
17h50-18h40	**O19 - SACI Gold Medal 2024: Kenneth Ozoemena** Electrifying Chemistry for clean and affordable energy in Africa
18h40-20h30	Ice breaker *Venue: Solomon Mahlangu Concourse*

Legend:

Plenary (no Q&A)	60 mins
Keynote Speakers (incl. Q&A)	50 min
SACI GOLD Medal Awardees (incl. Q&A)	45 min
SACI Raikes and Education Awardees (incl. Q&A)	30min
Invited (incl. Q&A)	30 min
Standard talk (incl. Q&A)	20 mins
Activities	

01-December 2025 – Monday morning

	Parallel A	**Parallel B**	**Parallel C**	**Parallel D**
08h00-08h50	**REGISTRATION**			
08h50 **PLENARY SESSION** (WSS2)	**O1 - Amanda Bryant-Friedrich** Posttranscriptional modifications in RNA: Where and why? **(O4)** Chair: Nicoletta Bathori			
10h00	TEA (Flower Hall) and move to sessions			
Chair Venue	Patricia Forbes WSS2	Memory Zimuwandeyi WSS3	Andrew Swarts WSS4	Nikoletta Bathori WSS5
10h30	**O38 - Midhun George** Development of a novel instrument for long-term measurements of OH reactivity)	**O47 - Remofilwe Manye** Investigating the pharmacological potential of ferrocenylbenzimidazole complexes as antimalarial and anticancer agents	**O56 - Robert Carroll** Electron nano-analysis of MOF glasses	**SPECIAL SESSION** (Elsevier): AI-Driven Innovations in Chemistry with Reaxys: Future Perspectives and Digital Transformation (Includes a discussion about how to support young chemists))
10h50	**O39 - Maki Mahlangu** Quantification and treatment of problematic odour-causing compounds in drinking water within Magalies Water Treatment systems and interrelated catchments	**O48 - Faith Akwi** A modular continuous flow synthesis of primaquine diphosphate an anti-malarial drug	**O57 - Tracy Lau** Topochemical postulates in action: comparative analysis of solid-state Diels-Alder reactions between similar charge transfer co-crystals	
11h10	**O40 - Ramasehle Moswane** Assessment of selected potential toxic elements and risk associated during seasonal variation at Hennops River, South Africa	**O49 - Pathy Lokole** Eco-friendly extraction of saponins from the leaves of *Musa paradisiaca* and their formulation into micelles for the co-encapsulation of antimalarial drugs	**O58 - Daniella Recchia** Extremely effective separations of pyridine/picoline mixtures through supramolecular chemistry employing TADDOL6 as the host compound	
11h30	**O41 - Sabetha Mapetla** Investigating the occurrence of pharmaceutical residues in urban estuarine water using grab and passive sampling approaches with UHPLC Q-Orbitrap MS analysis – A case of Durban Marina, South Africa	**O50 - John Mack** The photodynamic antimicrobial and anticancer activity properties of porphyrin, corrole, chlorin and N-confused porphyrin complexes	**O59 - Dave Billing** Crystallographic characterization of solid oxide electrolytes	
11h50	**O42 - Vhodaho Nevondo** Understanding the environmental impact of SCCPs: detection in consumer products, landfill leachate, and sediments from Gauteng	**O51 - Stacey Roman** Polymeric encapsulation of artemisinin-ferrocene hybrids as a route towards enhanced antimalarial delivery	**O60 - Nabanita Chatterjee** Substantial impact of ligated solvents on the degree of interpenetration controlling CO_2 and water sorption hysteresis in isoreticular MOFs	
12h10 (WSS2)	**O21 - SACI Raikes Medal 2025: Malik Dilshad Khan** Molecular precursor strategies for solid solutions and high-entropy materials in electrocatalysis Chair: Jan Weigand			

01-December 2025 – Monday afternoon

	Parallel A	**Parallel B**	**Parallel C**	**Parallel D**
Chair Venue	Sheldon Sookai WSS2	Andrew Swarts WSS3	Grace Ngubeni WSS4	Jan Weigand WSS5
14h00	**O7 - Annegret Stark** Sugarcane-derived lignin valorisation in material production for South Africa	O27 - **Robert Mokaya** Rational routes to porous carbons for sustainable energy applications (30min)	**O8 - Priscilla Baker** Signalling and measurement of small organic molecules in the context of health monitoring and well-being	**O9 - Cornie van Sittert** Modelling a sustainable energy future: NWU’s computational approach
14h55	**O43 - Akinshola Akinola** Magnetically-derived pecan nutshells for the removal of cadmium: artificial neural network modelling and photodegradation of sulfamethoxazole.	**O52 - Henrietta Langmi** Synthesis and evaluation of waste-derived metal-organic frameworks for hydrogen storage	**O61 - Anati Vitshima** Application of BSA-conjugated AgInS/ZnS QDs for electrochemical sensing of vascular endothelial growth factor	**O64 - Matthew Quesne** Computation for a green future: exploring the catalytic conversion of methane
15h15	**O44 - Jonathan Mukanya** Bioprospecting phytochemicals from banana plant wastes mediating green synthesis of metallic nanoparticles	**O53 - Carol Langa** Green synthesis of cerium/carbon-modified nis nanoparticles using *Sutherlandia frutescens* for photocatalytic dye degradation	**O62 - Clever Ng'andu** Calixarene-conjugated carbon dots for selective fluorometric detection of targeted pharmaceutical compounds in water	**O65 - Menezi Tshaka** Computational study of azobenzenes as cholesterol lowering drugs
15h35-16h00	**TEA (Flower Hall)**			
16h00	**O45 - Thabang Lebepe** Household microwave-assisted green synthesis of biocompatible gold nanostructures using *Aloe Africana* for biomedical applications	**O54 - Oluchi Nkwachukwu** Synthesis route matters: Interrogating the structural, morphological, optical, surface, photoelectrochemical and photocatalytic properties of lanthanum ferrite perovskite	**O63 - Benneth Iwuoha** Microwave-assisted synthesis of MOF-NiNPs@C for the electrochemical detection of Tramadol	**O66 - Morad El-Hendway** Computer-aided catalyst design: organic catalysts for CO_2 conversion into urea
16h20	**O46 - Bavuyile Magqira** Harnessing raw and the magnetised fly ash as low-cost adsorbents for the removal of pharmaceuticals from wastewater: Isotherms and Kinetics	**O55 - Galilee Byamungu** Synthesis and evaluation of dosimetrics features of silica nanoparticles derived from *Musa paradisiaca* pseudostem		**O67 - Ngonidzas Ruwizhi** Half-sandwich pyrazolyl-functionalized Ru(II)-NHC complexes: synthesis, characterization, antibacterial and DFT studies
16h40-17h50	**Poster session (Flower Hall)**			
18h00-22h30	**Braai @ Sci Bono**			

2-December 2025 – Tuesday morning

	Parallel A	Parallel B	Parallel C	Parallel D
08h00-08h50	REGISTRATION			
08h20	**poster time - evaluation**			
08h50 **PLENARY SESSION** (WSS2)	**O2 - Peter Wasserscheid** Catalysis for chemical hydrogen storage – status, challenges, and opportunities Chair: Neil Coville			
10h00	TEA (Flower Hall) AND MOVE TO SESSIONS			
Chair Venue	Charles de Koning WSS2	Dave Billing WSS3	Cornie van Sittert WSS4	Nikoletta Bathori and Bice Martincigh WSS5
10h30	**O68 - Viola Okechikwu** Room temperature detection of aspergillus flavus volatile organic compounds under simulated conditions using GO and SnO2 NRs	**O77 - Wing Fu Lai** Development of multifunctional polymeric materials for controlled release in food and pharmaceutical applications	**O87 - Werner van Zyl** Exploring orthogonal ligand scaffolds for selective metal coordination	**SPECIAL SESSION** (SACI CDI Panel Discussion): Breaking barriers: Critical questions for the future of chemistry **Ale Palermo, FRSC**: Innovating Chemistry: Designing Labs for Disability Inclusion
10h50	**O69 - Mahleba Masivuye** Selective - recovery of palladium(II) using dithiol- and benzimidazolylthio-functionalized merrifield resins	**O78 - Mahmood Patel** Critical differences in analytical techniques for the analysis of mercury in waste for landfill disposal assessment	**O88 - Nejat Habib** Metal-organic frameworks from environmentally benign synthesis for hydrogen and carbon dioxide storage	
11h10	**O70 - Mpelegeng Bvumbi** Photoisomerization, rotameric conformational behavior, computational insights, and antiplasmodial activity of cinnamoyl–chloroquine hybrids	**O79 - Pradish Rampersadh** Development of the multi-purpose reactor and the associated beamline facilities at the South African Nuclear Energy Corporation	**O89 - Monika Nowakowska** Salicylaldehyde cobalt–Schiff base complexes: balancing cytotoxicity and albumin pharmacodynamics for next-generation therapeutics	
11h30	**O71 - George Bepete** Solution-processed low-dimensional carbon materials via reductive dissolution	**O80 - Boitumelo Makume** The role of analytical chemistry in a decarbonising petrochemical industry	**O90 - Paula Maseko** From waste to catalyst: structural and catalytic evaluation of coordination polymers synthesized from PET via one-pot mechanochemistry for efficient dye removal from water	
11h50	**O72 - Lisa Myburgh** Design and synthesis of thiocarbonyl analogues of coumarin-based chemosensors with colourimetric properties: switching the selectivity from Fe^{2+}/Fe^{3+} to Hg(II) and Cu(II) ions	**O81 - Nikisha Sewpersad** Nanosilane-modified bitumen-stabilized base materials: mechanisms and moisture durability	**O91 - Andrew Swarts** Ligand design strategies to optimize hydrogen production via Ru-catalysed formic acid dehydrogenation	
12h10-12h30	**O25 - Jan Weigand** Molecularly tuned 4-phosphoryl pyrazolones for lithium recovery and selective rare earth extraction (30 min)	**O82 - Nestor van Eeden** Key aspects of pressurised water reactor (PWR) chemistry for safe and reliable operation	**O26 - Michael Nolan** Atomistic simulation of atomic level processing chemistries for materials deposition and etch (30 min)	
12h45-14h00	**Group Photo** **Lunch (& Council Lunch)**			

2-December 2025 – Tuesday afternoon

	Parallel A	**Parallel B**	**Parallel C**	**Parallel D**
Chair Venue	Pierre Mubiayi WSS2	Dave Billing WSS3	Bice Martincigh WSS4	Görkem Mergen and Sacha Devillers WSS5
14h00	**O10 - Martin Brits** Quantitation of micro and nanoplastics in human blood by pyrolysis-gas chromatography–mass spectrometry	**O11 - Xolani Nocanda** Detection, quantification and removal efficiencies of pharmaceutical contaminants in selected wastewater treatment plants at eThekwini Municipality	**O28 - Narayanaswamy Jayaraman** Remote activation route to access glycosyl cation – the case of 3-thiocresyl-prop-1-enyl (TCP) glycosides (30 min)	**SPECIAL SESSION** (ACS Presentation): Have you considered using CAS SciFinder® to support your job search or explore graduate programs?
14h55	**O73 - Christina Kannigadu** Untangling complexity in cola beverages: a non-targeted GC-TOFMS approach to volatile profiling and unexpected contaminant detection	**O83 - Adam Shnier** Rietveld refinement automation for process feedstock quality control (AUTO-INP) and other odd projects	**O92 - Simon Mnyakeni** Synthesis of sulfonylthioureas as potential antidiabetic drugs	
15h15	**O74 - Malesole Bucibo** Determination of heavy and polycyclic aromatic hydrocarbons in soil samples Witbank, South Africa	**O84 - Ryan Walmsley** Production of sustainable aviation fuel from Fischer-Tropsch wax - understanding the interplay between product properties and product yield	**O93 - Bridget Mtetwa** Development of norbornane-based compounds as MAO-B inhibitors for the treatment of Parkinson's disease	
15h35-16h00	**TEA (Flower Hall)**			
16h00	**O75 - Samukelisiwe Nhlapho** Non-targeted profiling of volatile compounds for the authentication of honey origin	**O85 - Andrew Venter** Beam line facilities at Necsa and their progression into the new multi-purpose reactor for material's analysis	**O94 - Temitope Olalekan** Synthesis, characterization and cytotoxicity of aminothiazole Schiff base and metal complexes	
16h20	**O76 - Mathew Khumalo** Development and application of "selective capture" derivatizing protocol for alcohols	**O86 - Izak Kotze** Silica-anchored acylthiourea and amine adsorbents for the selective recovery of platinum and palladium from aqueous media	**O95 - Vitalis Mbayo** Leveraging quantum mechanical and machine learning technologies for predictive modelling of Soursop (*Annona muricata Linn.*) phytochemical extracts against breast cancer	
16h40-17h50	**Poster session (Flower Hall)**			
18h00-22h30	**Periodic Pursuits (Science Stadium)**			

3-December 2025 - Wednesday

	Parallel A	Parallel B	Parallel C	Parallel D
08h00-08h50	REGISTRATION Science stadium			
08h20	**poster time - evaluation**			
08h50 **PLENARY SESSION** (WSS2)	**O3 - Greg Scholes** From coherence in photosynthesis to chemical quantum information science Chair: Andrew Forbes			
10h00	TEA (Flower Hall) AND MOVE TO SESSIONS			
Chair Venue	Songeziwe Ntsimango WSS2	Izak Kotze WSS3	Pierre Mubiayi WSS4	Chair: Andrew Forbes WSS5
10h30	**O96 - Thrineshen Moodley** The formulation of a novel chloroquinoline derivative in an amorphous solid dispersion and the determination of its thermal and solubility parameters	**O101 - Masego Ramonyai** The role of dipicolinic acid in enabling the simultaneous voltammetric analysis of copper and bismuth.	**O106 - Nomaswazi Madonsela** Effect of pyrolysis temperature of *Kigelia africana* biochar for the adsorption of lead(II) ions from aqueous solution	**SPECIAL SESSION** Chemistry and Quantum Science **Tjaart Kruger**: Manipulating individual light-harvesting complexes with light **Thomas Konrad**: TOPIC SAQuTI Panel Discussion
10h50	**O97 - Sarah Wright** Nucleophilic reactions of cyclobutenones	**O102 - Indiphile Nompetsheni** CQD-TiO$_2$ composite as a potential crypto-electrode modifier for high-performance aptasensing with ultra-low detection limit	**O107 - Cresten Moodley** Investigating the efficiency of transition and lanthanide-metal based coordination polymers for methylene blue adsorption	
11h10	**O98 - Marwaan Rylands** In search of the resurrection plant metabolite 3,4,5-tri-O-galloylquinic	**O103 - Kabelo Banda** Synthesis and characterization of mono, bi and tri composite of Ag, ZnO and MWCNT modified SPC electrode	**O108 - Dipuo Kgabi** Organobentonite–Ag/TiO$_2$ composite for Cr(VI) removal and bacterial disinfection	
11h30	**O99 - Aviwe May** Effects of structural modification on established BODIPY dye properties for modern applications	**O104 - Racheal Ijimdiya Ukachi** A comparative material-performance study of sulphur-and phosphorous-doped reduced graphene oxides for electrochemical biosensing of organophosphorus pesticides	**O109 - Sifiso Nsibande** Quantum dot-based sensors: synthesis, characterization and application for the detection of organic pollutants in environmental samples	
11h50 - 12h10	**O100 - Memory Zimuwandeyi** Towards the synthesis of hydroxylated polyamines	**O105 - Funmilola Adesanya** Carbonization of hemp-derived carbons: a comparative study of activation routes	**O110 - Sifelani Dube** Reduced graphene oxide–ion imprinted polymer (RGO nanocomposite sensor: tackling cadmium pollution in water	
12h30 (WSS2)	**O20 - SACI Gold Medal 2025: Egmont Rohwer** The joy of research in separation science Chair: Patricia Forbes			
13h20	Lunch and Excursion			

4-December 2025 – Thursday morning

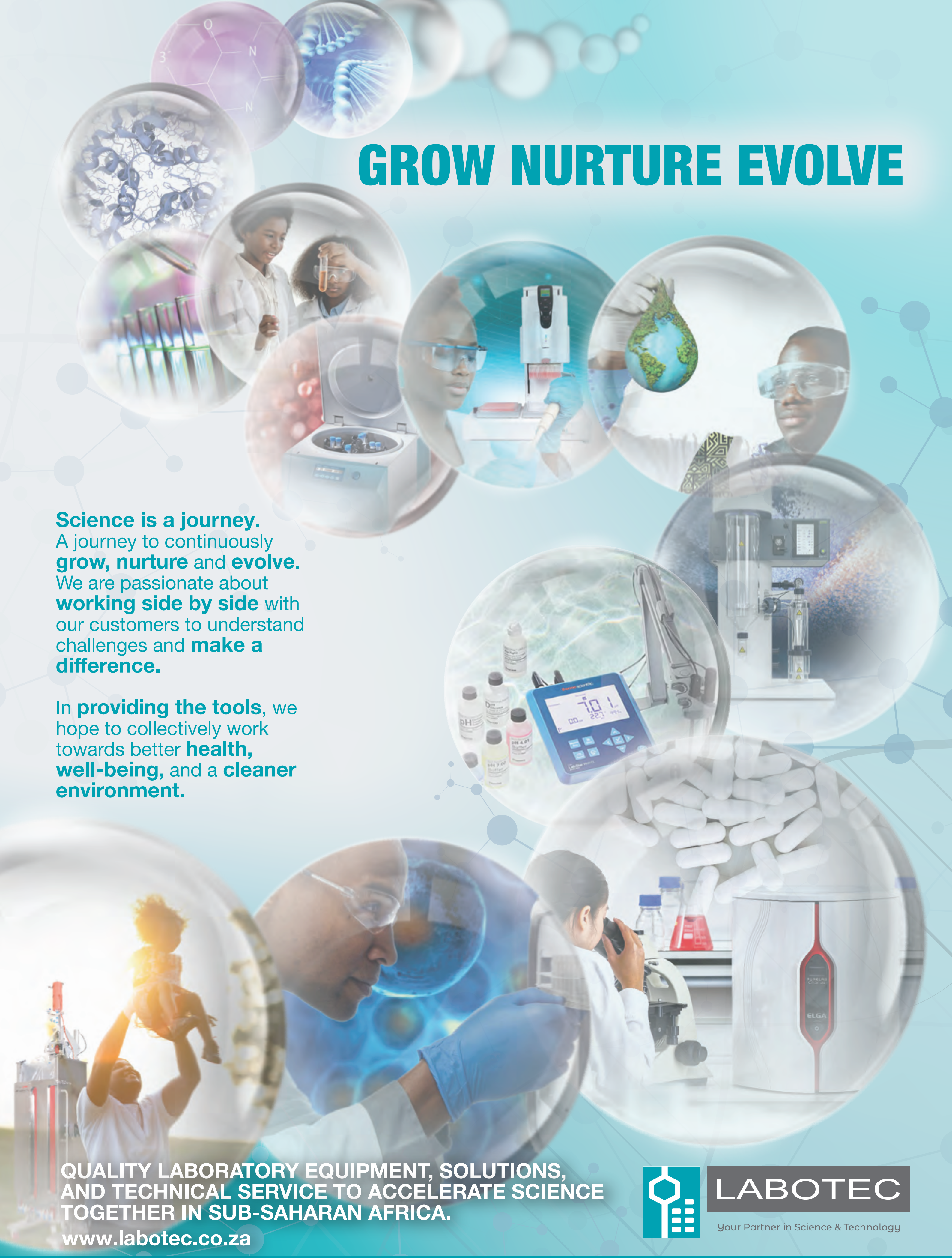
	Parallel A	Parallel B	Parallel C	Parallel D
08h00	REGISTRATION			
08h20	**poster time - evaluation**			
08h50 **PLENARY SESSION** (WSS2)	**O4 -Margaret Blackie** How we think about what we do matters: Developing a model to underpin chemistry education Chair: Caren Billing			
10h00	TEA (Flower Hall) AND MOVE TO SESSIONS			
Chair Venue	Grace Ngubeni WSS2	Zenixole Tshenu WSS3	Vincent Nyamori WSS4	Marietjie Potgieter WSS5
10h30	**O111 - Mothusi Molebatsi** MOF-functionalized nanocellulose from *Agave Sisalana* plant for efficient copper removal from treated wastewater	**O119 - Oluwatoyi Akerele** Analysis of the structural and energetic properties of carbofuran and its polymorphs	**O127 - Adeniyi Ogunlaja** Catalytic performance of nanostructured Fe_x–$Mo_{0.1}$ /TiO_2–Al_2O_3 Systems in dibenzothiophene hydrodesulfurization	**O135 - Comfort Nkambule** From undergraduate organic chemistry to functionalized heterocycles
10h50	**O112 - Lelethu Kontile** Exploration of plant *Eucalyptus cinerea* essential oil as a green, affordable, and sustainable adsorbent for the removal of antibiotics from wastewater	**O120 - Andreas Lemmerer** A tale of two polymorphic pharmaceuticals: the solid state organic chemistry of persedon and propylphenazone	**O128 - Abongile Gingqi** Sustainable conversion of waste cooking oil to biodiesel using bifunctional metal-supported MOF-based heterogeneous catalysts	**O136 - Lynne Pilcher** Systems thinking for sustainability in chemistry education using green chemistry metrics and life cycle inventories of aspirin synthesis
11h10	**O113 - Sello Moloi** Fluoride removal from water by the application of bone char prepared from wild animal and bird bones	**O121 - Jarryd Vorgers** Peroxides as host compounds: an investigation of the host ability and selectivity of di-(9-(p-trifluoromethylphenyl)xanthen-9-yl peroxide in mixed anisole/methylanisoles	**O129 - Sheldon Sookai** Biophysical studies of metal chelate binding by HSA: towards an understanding of metallodrug transport	**O137 - Shaeen Chetty** Beyond the Curve: unpacking molar absorptivity in HPLC
11h30	**O114 - Eric Danso-Boateng** Adsorbents derived from invasive weeds for pollutant control	**O122 - Babatope Ojo** Integrated Z-scheme BiOCl/$NiTiO_3$ heterostructured photoanode and its photoelectrocatalytic application in ciprofloxacin degradation	**O130 - Wilson Seleka** Advancing electrocatalysis: a comprehensive review of metal (Cu, Co, Ni, etc) nitrides, sulphides, and phosphides for nitrate reduction reaction (NO_3 RR) to ammonia an alternative energy carrier	**O138 - Winifred Esiefa** Innovative teaching strategies for sustainable chemical education
11h50	**O115 - Naom Momanyi** Magnetic carbon nanosheets derived from PET plastic waste for the preconcentration and adsorptive removal of selected trace metals in water	**O123 - Atiyyah Salajee** Polymorphism In ternary complexes	**O131 - Pierre Mubiayi** Nanocrystalline perovskite: the last man standing	**O139 - Marissa Rollnick** Understanding the long-term development of high school teachers' insights into their PCK of chemical bonding
12h10 (WSS2)	**O24 - Merck Medal: Lawrence Madikizela** Pharmaceuticals as chemicals of emerging concern in East London major estuaries and seawater			
12h45 (WSS2)	**O23 - SACI Education Medal 2024: Liliana Mammino** Chemistry as an ideal central area for sustainability-related multidisciplinary Chair: Helen Drummond			
13h20-14h00	Lunch			

4-December 2025 – Thursday afternoon

	Parallel A	**Parallel B**	**Parallel C**	**Parallel D**
Chair Venue	Willem van Otterlo WSS2	Monika Nowakowska WSS3	Songeziwe Ntsimango WSS4	Megan Matthews WSS5
14h00	**O12 - Ron Heeren** Mass spectrometry in Spatial Biology: Imaging, single cells and translational life sciences		**O13 - Vladimir Azov** Expanding peptide chemical space: functional non-canonical amino acids for smart soft materials	**O14 - Marietjie Potgieter** Embedding Relevance, Values and Identity in Chemistry Education
14h55	**O116 - Mufaro Mugari** Gas chromatography for decision-grade evidence in cannabis labelling and human pesticide exposure	**O124 - Cyprian Moyo** Python-based quantum chemistry software in the era of quantum computing: educational tools, platforms, and research integration	**O132 - Chakes Mashaba** Design and synthesis of 8-quinoline-1,3,4-oxadiazole-thio-acetamide and ethanone derivatives as potential anti-HIV agents	**SPECIAL SESSION** (Chemistry Education Panel Discussion): Shaping the future of education in Analytical Chemistry
15h15	**O117 - Lethabo Masemola** Phytochemical investigation and biopharmaceutical profiling of secondary metabolites from *Pappea capensis* for anticancer properties	**O125 - Jurgens de Langa** Molecular-wide chemical bond theory: bridging the gap between atomistic chemistry and holistic physics	**O133 - Blesant Maluleke** Synthesis and biological evaluation of quinoxaline derivatives as potential anti-tuberculosis agents	
15h35 – 15h55	**O118 - Ntsieni Molaudzi** Photodegradation Kinetics of Amoxicillin, Carbamazepine and Diclofenac Under Simulated Solar Light: Fluorescence EEMs Deconvolution Insights	**O126 - Divya Pant** Impacts of aromatic bridges on electronic and nonlinear optical properties of Reichardt's types of zwitterionic molecules: a computational study	**O134 - Lebogang Mabatamela** Design and synthesis of pyrazolopyrimidine, pyrazolopyridine pyrrolopyridine, and pyrrolopyrimidine derivatives as potential anti-malaria agents	
16h00-16h30	**TEA (Flower Hall)**			
16h30-17h05 (WSS2)	**O29 - Ehud Keinan** Humanity faces a bright future, and so Chemistry (30 mins) Chair: Bice Martincigh			
18h00-23h00	**Travel and Gala Dinner (Thabo Eco Hotel)** – *Casual*			

5-December 2025 - Friday

	Parallel A	**Parallel B**	**Parallel C**
08h50 **PLENARY SESSION** (WSS2)	**O5 - Christian Klampfl** Reclaimed waters for irrigation: how plants interact with drug residues Chair: Ale Palermo Venue: WSS2		
10h00	TEA (Flower Hall) AND MOVE TO SESSIONS		
Chair Venue	Izak Kotze WSS2	Sheldon Sookai WSS3	Monika Nowakowska WSS4
10h30	**O15 - Vincent Nyamori** Carbon-based nanocomposites for fourth - generation solar cells	**O16 - Perdita Barran** Weighing molecules to treat and diagnose disease, from viruses to skin swab	**O17 - Moniek Tromp** The quest for sustainable and circular battery technologies - operando x-ray techniques probing dynamic processes in batteries
11h25	**O140 - Sense Mametja** Construction of oxygen deficient NiAl-LDH-nanocomposites for enhanced photocatalytic hydrogen evolution via water splitting	**O143 - Nare Mojela** *Moringa oleifera* and Marula derived platforms for bioanalytical and biomedical applications	**O145 - Gwibaka Feleni** Innovative inner transition metal-MXene anodes for high performance sodium-ion batteries
11h45	**O141 - Mbali Moreki** Exploring morphology-dependent photocatalysis of ZnO nanoparticles towards rhodamine 6g degradation under UV light	**O144 - Tatenda Machakaire** From leaves to leads: Uncovering potential COX-2/5-LOX dual inhibitors from South African medicinal plants	**O146 - Agustus Lebechi** Hybrid bifunctional FeCo-Fe_2CoO_4 electrocatalyst supported on carbon conducting agent For high areal discharge energy rechargeable zinc-air battery
12h05	**O142 - Samantha Ndlovu** Enhancing dye-sensitized solar cell performance by introducing Fe/Co into the B-site of $Sr_{0.7}Sm_{0.3}BO_{2.89}$ perovskite photoanodes		**O147 - Aderemi Haruna** Investigation of high entropy manganese-based fluorophosphate electrocatalysts for electrocatalytic and energy storage applications
12h25 (WSS2)	**O22 - SACI Raikes Medal 2024: Maya Makatini** From molecular adventures to wellness: Translating peptidomimetics and mass spectrometry into therapeutic and diagnostic innovations Chair: Charles de Koning		
13h00	**Prize giving/Closing** WITS Science Faculty Dean: Nithaya Chetty (10 min) FASC rep: Vincent Nyamori (5 min) Comm Chem rep: Ale Palmero (5 min) ACS rep: Charles de Koning (5 min) SACI EXCO: Caren Billing (5 min) Chair: Manoko Maubane-Nkadimeng		
Lunch, (packed lunch) **End of conference/Travel**			



Posttranscriptional Modifications in RNA: Where and Why?

Amanda Bryant-Friedrich[a]

[a]Department of Pharmaceutical Sciences, Wayne State University, 259 Mack Avenue
Detroit, Michigan 48201, United States of America, E-mail: Amanda.bryant-friedrich@wayne.edu.

Keywords: ribonucleic acids, methylation, pseudouridine, oxidative damage

Post transcriptional modifications in RNA play a very significant role in lending stability to RNA constructs, preparing them for export from the nucleus, participation in translation by ribosomes, and gene expression. These modifications vary significantly depending upon the type of RNA and its function. A significant role of post transcriptional modifications in RNA is to modulate the cellular response to stress. To date well over 100 modifications to RNA at the bases and the sugars have been identified. The role of these modifications in biological processes has been often investigated and, in some cases, their extensive impact on processes elucidated. To fully understand the role of post transcriptional modifications in RNA a full map of the epitranscriptome is required and elucidation of the role of all modifications, their locations and their impact on stability and structure is required.

To reach this goal tools must be developed which are reliable and standardized in a way that makes experimentation reproducible and applicable to various platforms. The synthesis of modified nucleosides and oligonucleotide containing suspected and verified post transcriptional modifications has been accomplished. These tools have been used to investigate the impact of post translational modifications on RNA structure chemical stability and stability towards oxidative stress. The synthesis of tools for the investigation of O6-methyl guanine and pseudouridine modifications will be discussed.

Catalysis for chemical hydrogen storage – status, challenges, and opportunities

Peter Wasserscheid[a,b]

[a]Lehrstuhl für Chemische Reaktionstechnik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstrasse 3, 91058 Erlangen, Germany; peter.wasserscheid@fau.de
[b]Forschungszentrum Jülich, Helmholtz-Institut Erlangen-Nürnberg (IET-2), Cauerstraße 1, 91058 Erlangen, Germany & Reaction Engineering for Chemical Energy Storage (INW-3), Institute for a Sustainable Hydrogen Economy, Marie-Curie-Straße 5, 52428 Jülich, Germany; p.wasserscheid@fz-juelich.de

Keywords: hydrogen, hydrogenation, dehydrogenation, catalyst development, kinetics

Global logistics of renewable energy equivalents will create additional driving force towards a future hydrogen economy. However, the special nature of H_2 requires dedicated infrastructures (high pressure or cryogenic) and this has prevented so far its massive introduction to the energy sector.

Recent scientific and technological progress in handling hydrogen in chemically bound form supports the technological vision that a future hydrogen economy may work without handling large amounts of elemental hydrogen using the existing infrastructure for fuels. Liquid Organic Hydrogen Carrier (LOHC) systems are composed of pairs of hydrogen-lean and hydrogen-rich organic compounds that store hydrogen by repeated, catalytic hydrogenation and dehydrogenation cycles.[1] CO_2- and biomass-based LOHC systems add interesting features to the more traditional systems based on aromatic/heteroaromatic compounds and their perhydro counterparts.[2]

The contribution will highlight fundamental and applied aspects of LOHC hydrogenation and dehydrogenation catalysis and the related processes. It will focus on the development of optimized catalytic materials for LOHC hydrogenation/dehydrogenation reactions,[3,4] and on operational stability aspects gained from demonstration units.[5,6] Application scenarios and implementation timelines for stationary energy storage systems, hydrogen logistics and mobile applications will be discussed.

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From coherence in photosynthesis to chemical quantum information science

Gregory D. Scholes

[a]Princeton University, New Jersey, 08544, United States; E-mail: gscholes@princeton.edu

The parallel and synergistic developments of atomic resolution structural information, new spectroscopic methods, their underpinning formalism, and the application of sophisticated theoretical methods have led to a step function change in our understanding of photosynthetic light harvesting. These new spectroscopic methods, in particular multidimensional spectroscopies, have enabled a transition from recording rates of processes to focusing on mechanism. Such studies indicated the possibility that advanced ultrafast techniques can give insights into the time evolution of the density matrix of the system. I will explain the story of how our understanding of these experiments evolved [1].

This work led to the question of how coherence in chemical systems can be leveraged for function [2]. I will discuss coherence and its role in ultrafast chemical reactions. I will report experiments that illustrate how vibrational wavepackets can serve as a molecular-scale probe to give insight into the reaction coordinate of electron transfer reactions. Valuable insights into electron transfer reactions have been established using Marcus theory. However, a complementary theoretical model explaining how vibrational wavepackets evolve during electron transfer reactions has not yet been established. I will describe a “quantum quench” model to address this gap.

We then ask, how might related developments enable advances in quantum information science? A defining characteristic of molecules is that they are intrinsically complex quantum systems with many degrees of freedom, exhibiting remarkable variety. Molecules, therefore, have different quantum properties than atomic systems, including solids. Our aim in in chemical quantum information science (QIS) should then be to leverage these distinctions. This is where transformative advancements lie. I will outline and motivate the QIS “wish list” for chemistry that we described in a recent report [3].

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Utilizing Coherence to Enhance Function in Chemical and Biophysical Systems
[3] Gregory D. Scholes, Alexandra Olaya-Castro, Shaul Mukamel, Adam Kirrander, Kang-Kuen Ni,Gordon J. Hedley, and Natia L. Frank, J. Phys. Chem. Lett. **16**, 1376−1396 (2025).
The Quantum Information Science Challenge for Chemistry

How we think about what we do matters: Developing a model to underpin chemistry education

Margaret Blackie[a]

[a]Center for Advancing Undergraduate Science Education, Virginia Tech, Blacksburg, Virginia, 24060, USA E-mail: magsblackie@vt.edu.

Keywords: evaluative judgement, epistemic assessment framework, nature of science, disciplinary knowledge

Good undergraduate chemistry education requires more than covering the content required by the accrediting body. Meaningful engagement with disciplinary knowledge is essential for the training of a professional chemist. Evidence from a seven year longitudinal study suggests that graduates who have more sophisticated views of their discipline are more likely to end up in graduate level employment regardless of whether they are employed within their discipline.[1] As generative AI continues to evolve, graduates are likely to be required to move into areas beyond their primary degree. The data seems to suggest that deep engagement with disciplinary knowledge sets students up for life-long learning. The question we then must ask is how we enable this deep engagement with knowledge.

In this paper I will synthesize the work I have done in chemistry education over the last 15 years. I will introduce a model which includes disciplinary knowledge, the nature of the discipline, meaningful assessment practices and the development of evaluative judgement.[2] This draws on the development of the epistemic assessment framework.[3] The understanding of the practice of chemistry to be an interplay between the canon of chemistry, a community of chemistry and the world at a molecular level.[4] It requires a grappling with the nature and purpose of education.[5]

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Reclaimed waters for irrigation: how plants interact with drug residues

Christian W Klampfl[a]

[a]Institute of Analytical and General Chemistry, Johannes Kepler University Linz, Altenbergerstrasse 69, A-4040 Linz, Austria, E-mail: Christian.klampfl@jku.at

Keywords: treated wastewater, water re-use, emerging contaminants, plant uptake, metabolization

Water policy is a major topic worldwide and consequently also within the European Union (EU), resulting in a number of directives (e.g. 2008/105/EC, 2013/39/EU) focusing on the aim of guaranteeing a good water quality. In addition, the EU campaign “Water is too precious to waste“, points out the problem of water shortages and droughts across the EU in the recent years. Water scarcity already affects more than 10 % of the population in Europe and almost 20 % of the EU territory respectively. Consequently, by the year 2030, 50% of Europe’s river basins might be affected by this issue [1,2]. For this reason, the re-use of treated wastewater (TWW), wherever possible, can be understood as an important step for fighting water scarcity. TWWs are mostly used in agriculture, as the percentage of cultivable surface requiring irrigation for successful farming is continuously growing. Countries like Malta and Cyprus where 90 % and 60 % respectively of the TWW is re-employed are in the forefront of water re-use – when focusing on the European continent. More countries of the European south, reuse between 5 and 12 % of their TWW only, leaving a huge potential for improvement [2].Modern wastewater treatment plants succeed in the removal of more and more pollutants from the wastewater. The trend of installing an additional (fourth) stage to these plants can be seen as an important step towards a continuous improvement of both the treatment plant design and the processes employed therein. Nevertheless, TWW still may contain a variety of micropollutants with pharmaceuticals and personal care products (PPCPs) being a prominent sub-fraction within this group.

In this talk strategies to investigate the interaction of such pollutants with plants (when contaminated water is employed for irrigation) will be presented. These range from the use of cell cultures as model substances over in-lab cultivation of selected model plants (commonly using hydroponic systems) to field studies with crops being irrigated with actual reclaimed waters. Thereby uptake and further biotransformation for a range of contaminants, spanning from typical personal care products (e.g. sunscreens) to widely prescribed pharmaceuticals such as non-steroidal anti-inflammatory drugs, b-blockers, anti-depressants and pain killers will be discussed. A particular focus will be set on the transport of these substances within the plants (from root to stem, leaves and fruit) as well as the formation of drug-derived metabolites [3,4]. Growing experiments were conducted using actual TTWs as well as in-lab mixed artificial wastewater samples for studying particularly the biotransformation of these substances within a range of plants used for the production of food and feed (e.g. lettuce, tomato, maize, pea, amaranth, rice) [5].

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Everyone can innovate

David Fine

Keywords: Innovation

Everyone is born with the innate ability to innovate. Pre-school children playing in a sand box imagine one wooden block to be a car and another a house and another a fire engine. When we think of Innovation, five words that come to mind are Brilliance, Genius, Expertise, Success and Praise. These perceptions are way off the mark. In my personal experience as a serial innovator, I found that (i) Tenacity and hard work, called Grit, are far more important than Brilliance. (ii) Serendipity (luck) always outperforms Genius. (iii) Experts know too much to have brand new ideas whereas naïve newcomers think clearly and can innovate. (iv) Failure is an essential prerequisite for Success. (v) Instead of Praise, expect fierce criticism and withering personal attacks when your innovation is successful, especially if it works despite accepted dogma. I also found that diversity in cultural upbringing and training often helped to stimulate innovation.

Sugarcane-derived lignin valorisation in material production for South Africa

Annegret Stark, Josiane Ayingeneye, Justice Mphahlele, Nomfundo Ndlovu and Kiaran Govender

SMRI/DSTI/NRF SARChI Chair Sugarcane Biorefining in South Africa, Discipline of Chemical Engineering, University of KwaZulu-Natal, Durban, South Africa, E-mail: starka@ukzn.ac.za.

Keywords: sugarcane bagasse, organosolv lignin, material production and properties

The beneficiation of industrial residues is a major aspect of the *South African Sugarcane Value Chain Master Plan to 2030*, to diversify and economically stabilise this industry of national importance. Most focus is placed on chemicals, although several materials that can be derived from sugarcane, and in particular from its bagasse, could serve both local and international industries such as packaging, automotive and constructions. As a developing country, South Africa possesses a vast potential of economic growth in these as well as the energy and consumer products sectors, and our work seeks to unlock these markets.

In South Africa, the Illovo Sugar company operates a steam explosion process generating furfural and other products from the hemicellulose contained in bagasse. The residue of this process is a fine powder consisting mostly of cellulose and lignin. It is currently used as fuel in the sugar mill boilers providing process energy. However, have recently optimised an organosolv process to isolate lignin from this residue, which is easily accessible using mild conditions. The lignin was fully characterised, and applied as binder in three materials, addressing specific industry needs in South Africa:

Firstly, the local coal mining industry has to deal with a legacy of unused coal fines, which cause environmental concern, as fines can neither be transported nor used as fuel. We found that lignin exhibits suitable properties to act as a binder in the manufacture of briquettes.

Secondly, we have developed bagasse-based particle boards using lignin as binder, yielding eco-friendly materials with excellent properties. This is of interest since the industry needs to replace urea and phenol formaldehyde adhesives, which release toxic formaldehyde over time.

Thirdly, South Africa has recently made much progress in terms of the Extended Producer Responsibility Regulations, which seek to translate the current linear, take-make-dispose economy to a Circular Economy. Initial focus is placed on target wastes including electrical, electronic and lighting equipment, as well as paper, packaging and single use materials. One of the key issues in this context is to find outlets for recycled materials, such as polypropylene. We have produced composite materials using recycled polypropylene, bagasse and lignin, where the addition of lignin was shown to tremendously improve the materials' properties.

An overview of the current R&D efforts on the value-addition of lignin from sugarcane in materials will be presented. Technical aspects of the production of lignin from bagasse, and its characterisation, the development and production of the particleboards, composites and coal briquettes, will be discussed. Focus will be placed on the effect of lignin on the materials' properties and potential application areas. Finally, preliminary techno-economic indicators are discussed to highlight opportunities for sector-overarching industrial symbiosis.

Signaling and measurement of small organic molecules in the context of health monitoring and well-being

Priscilla G L Baker[a], *Clementine Louw*[a], *Teboho Moeketse*[a]

[a]SensorLab research group, Chemistry department, University of the Western Cape, Bellville, PB X17, South Africa,
Email: pbaker@uwwc.ac.za

The detection and analysis of small organic molecules play a pivotal role in advancing health monitoring and personal well-being. These molecules, including metabolites, hormones, and biomarkers, serve as critical indicators of physiological states and disease progression. Developments in biosensors, wearable devices, and lab-on-a-chip technologies have significantly improved the sensitivity, specificity, and temporal resolution of molecular detection. Coupled with advances in synthetic biology and nanotechnology, novel signaling strategies have enabled the precise tracking of biochemical changes in vivo and ex vivo. However, challenges remain in achieving robust signal transduction in complex biological environments, ensuring biocompatibility, and integrating multimodal sensing into scalable, user-friendly formats.

Continuous monitoring of small organic molecules using electrochemical sensor technology offers a transformative approach to personalized health management and real-time physiological assessment. This technology enables rapid, sensitive, and selective detection of key biomarkers directly from biological fluids like sweat and saliva. Using advanced carbon based nanomaterials and analytical expertise in separating and enhancing analytical signals, we have moved towards the selective and unambiguous detection of uric acid, cortisol, and dopamine. In this presentation we will have a closer look at the analysis and performance of prototype devices from our recent work.

Modelling a Sustainable Energy Future: NWU's Computational Approach

Cornie GCE van Sittert [a]

[a]Laboratory for Applied Molecular Modelling, Research Focus Area: Chemical Resource Beneficiation, North-West University, 11 Hofmann Street, Potchefstroom, 2531, South Africa

Keywords: energy materials, first-principles calculations, bimetallic, photovoltaics, batteries

The rapid advancement of energy technologies demands the development of high-performance materials for energy generation, storage, and conversion. Computational methods have emerged as powerful tools for accelerating the discovery, design, and optimization of these materials. This presentation explores the role of first-principles calculations and molecular dynamics simulations in predicting the structural and electronic properties of energy materials. Case studies will highlight breakthroughs in photovoltaics, batteries, and bimetallic materials, demonstrating how computational modelling enhances efficiency and sustainability. By integrating theory with experiments, computational approaches pave the way for next-generation energy materials with improved performance and durability.

Quantitation of micro and nanoplastics in human blood by pyrolysis-gas chromatography–mass spectrometry

Martin Brits[a,b], *Martin J.M van Velzen*[a], *Feride Öykü Sefiloglu*[a,c], *Lorenzo Scibetta*[a], *Quinn Groenewoud*[a], *Juan J. Garcia-Vallejo*[d], *and Marja H. Lamoree*[a]

[a]Amsterdam Institute for Life and Environment (A-LIFE), Faculty of Science, Vrije Universiteit Amsterdam, De Boelelaan 1108, 1081 HZ Amsterdam, the Netherlands. [b]The Southern African Grain Laboratory (SAGL), Grain Building-Agri Hub Office Park, 477 Witherite Street, The Willows, Pretoria, 0040, South Africa. [c]Netherlands Organisation for Applied Scientific Research (TNO), Utrecht, 3584 CB, The Netherlands. [d]Department Molecular Cell Biology & Immunology, Amsterdam University Medical Center (VUmc location), De Boelelaan 1108, 1081 HZ Amsterdam, the Netherlands

Keywords: Microplastics, Pyrolysis-gas chromatography mass spectrometry, Quantitation, Human blood

The detection of micro and nano-plastic (MNP) particles in blood revealed that microplastics are taken up in the human body and transported via the bloodstream [1,2]. These scientific findings received significant attention and impacted the understanding of human internal microplastic exposure. Although there is limited information on the effects of MNPs on human health, human exposure is evident by the detection of microplastics in drinking water, food, and air. The toxicity of MNPs may be influenced by multiple physical characteristics such as shape, size, and polymer type and composition. With the increased usage of plastic products, the levels of microplastics in our living environment are expected to increase in the coming years. The occurrence of MNPs in lung tissue supports human inhalation as a route of environmental exposure [3]. In addition, MNPs were also reported in human breastmilk [4] and human placenta [5], indicating that the unborn foetus and new-borns are exposed.

The quantitation of MNPs in biological matrices and their possible effects and interactions are still poorly investigated, mainly due to the lack of robust methods with a high degree of sensitivity and selectivity. Thermo-analytical methods coupled with mass spectrometry allow for the simultaneous, selective, and sensitive analysis of MNPs and permit quantification in addition to detection. Pyrolysis-gas chromatography coupled to mass spectrometry (Py-GC-MS) has been successfully applied for the detection of several polymers in environmental samples. Using this destructive method, MNP particles (size range larger than 700 nm) were recently analysed in human whole blood samples [2].

We present a robust and sensitive sample preparation and analytical method using Py-GC-MS To ensure the accuracy of the analytical method, method validation was performed using an in-house quality control (QC) sample spiked with six polymers (polyvinyl chloride (PVC), poly(methyl methacrylate) (PMMA), polypropylene (PP), polystyrene PS), polyethylene (PE) and polyethylene terephthalate (PET)). The method was applied to measure plastic particles in 68 human whole blood samples from healthy volunteers. The QC samples were included in batch analysis to assess the reproducibility. Results show that plastic particles were detected in blood and are therefore bioavailable for uptake into the human system. The exposure metrics and related hazards of these plastic particles in humans are needed to estimate the public health risks.

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Detection, quantification and removal efficiencies of pharmaceutical contaminants in selected wastewater treatment plants at eThekwini Municipality

Xolani Nocanda[a], *Jerker Fick*[b] *and Abdul Kaium*[b]

[a]Council for Scientific and Industrial Research, Meiring Naude Road, Brummeria, Pretoria, 0001, South Africa, E-mail: xnocanda@gmail.com , [b]Chemistry Department, University of Umea, Sweden.

Keywords: pharmaceutical, pollutants, contaminants of emerging concern, wastewater treatment works

Water plays a critical role in human life, animal life, economic growth and sustainable ecosystem. South Africa is rated as one of the driest countries in the world with an estimated yearly rainfall of 450 mm against the world yearly estimated rainfall of 860mm [1]. Challenges brought by climate change, population growth, urbanization and industrialization are causing stress to water supply. Furthermore, an increase in population, industries and new chemical products entering the market results in high levels of pollution in water.

Some pollutants in water are monitored and some are not. Pollutants that are not monitored but can negatively affect human life, aquatic life and the ecosystem are called Contaminants of Emerging Concern (CECs). Some of the known CECs are endocrine disrupting chemicals, disinfection by-products, pharmaceuticals contaminants, microplastics, pesticides, personal care products and nanomaterials. The study focused on pharmaceutical contaminants present in wastewater from selected wastewater treatment works at eThekwini municipality.

EThekwini municipality has initiated projects aimed at producing re-use water from wastewater for different purposes. To support the re-use projects, this study was initiated with the aim of detecting, quantify and work out removal efficiencies of pharmaceutical contaminants in wastewater from selected wastewater treatment works with different treatment processes. From the studied wastewater treatment processes, the best treatment process for removal of pharmaceutical contaminants in wastewater was revealed.

The following wastewater treatment works were selected for the study, Amanzimtoti wastewater treatment works (WWTW), Umbilo WWTW, KwaMashu WWTW, Southern WWTW, Northern WWTW, MEB pilot plant and Durban Water Recycling plant. MEB pilot plant and Durban water recycling plant are re-use plants, while other selected wastewater treatment plants are investigated for re-use projects.

Using LCMS/MS, a total of 39 pharmaceutical contaminants in wastewater were detected, quantified and removal efficiencies were calculated. Paracetamol and Lamivudine were detected in highest concentrations between 0.06 mg/L and 0.80 mg/L. The results showed excellent removal efficiency for the studied pharmaceutical contaminants at MEB pilot plant and at Durban Recycling Plant, above 80% removal between the influent and the final effluent. The re-use water produced at MEB pilot plant was produced for drinking purposes and was tested against set limits in the South African National Standard for drinking water (SANS241:2015) and complied, however the presence of CECs in re-use water and risk associated needs further investigations.

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KEYNOTE **O12**

Mass spectrometry in Spatial Biology: Imaging, single cells and translational life sciences

Ron M.A. Heeren and the whole M4i team[a]

[a]The Maastricht MultiModal Molecular Imaging institute, Maastrucht university, Universiteitssingel 50, 6229 ER Maastricht, The Netherlands, E-mail: r.heeren@maastrichtuniversity.nl

Keywords: Spatial biology, Mass Spectrometry imaging, multi-omics, single cell

Modern molecular analytical chemistry technologies in the “omics” arena plays an increasingly important role in clinical diagnostics. Technological advances have increased methodological sensitivity, allowing researchers to acquire detailed molecular information of smaller and smaller samples. The biggest challenge is to put that concerted information in the context of the biological problem the samples originate from. Innovative molecular imaging technologies at the single cell level, have impacted translational clinical research and beyond. Sensitive and selective molecular microscopes in modern spatial biology offer new insights in spatial and molecular complexity of cellular metabolism that contextualize cellular function in health and disease. Imaging mass spectrometry has firmly established itself as a key technology in spatial biology. It’s capabilities of revealing contextual, local molecular information on the microscale aid researchers to provide fundamental insights into biological processes related to health and disease.

One key aspect of translational clinical success is the ability to obtain this molecular information on thousands of molecules on a process relevant time- and length scale. Targeted and untargeted imaging technologies offer remarkable insights in the complexity required for systems medicine enabling diagnostics. Single cells can be analyzed in great molecular detail and in the context of their native tissue. Combined, this offers a true multi-omics approach that reveals contextual molecular complexity for patient stratification and personalized medicine. And it is analytical chemistry that lies at the basis of the interdisciplinary research needed to make it routinely happen in the future.

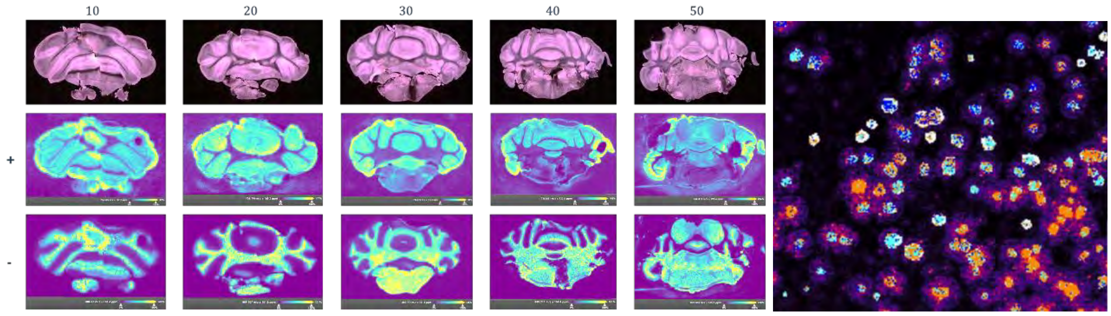


Figure 1. Reproducible and stable molecular pathology with MALDI-MSI across a mouse brain and a single cell multimodal image showing the molecular complexity of patient derived cell lines.

Expanding peptide chemical space: functional non-canonical amino acids for smart soft materials

Vladimir A. Azov[a], *Francois De Beer*[a], *Akho Ntsila*[a], *Adelaide R. Mashweu*[a],
Jolien Bertouille[b], *Charlotte Martin*[b], *Steven Ballet*[b], *and Ulrich Hennecke*[b]

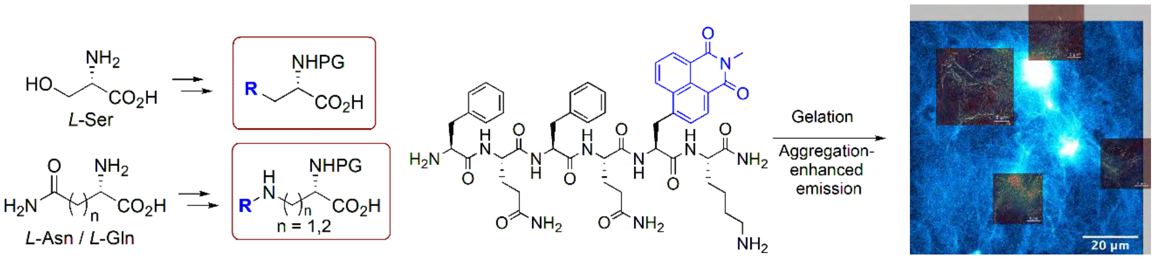
Department of Chemistry, University of the Free State, PO Box 339, Bloemfontein, 9300, South Africa, E-mail: azovv@ufs.ac.za. [b]Vrije Universiteit Brussel, Pleinlaan 2, 1050 Brussel, Belgium

Keywords: non-canonical amino acids, peptides, soft materials, hydrogelators, cross-coupling reactions

Only 22 natural α-amino acids are encoded by the genetic code and incorporated into proteins, inherently limiting the structural diversity of peptides that can be assembled from readily available, naturally derived starting materials. To expand the chemical space of peptide-based molecules, the synthesis of non-canonical amino acids (ncAAs), bearing substituents not found in nature, has become a vibrant area of research [1].

In our project, we focus on the synthesis of ncAAs featuring functional groups such as electron donor (D) and acceptor (A) moieties, as well as fluorescent and redox-active units. These modified amino acids are intended for use in materials science, where they can enhance weak intermolecular interactions of amino acids within peptides, ultimately improving structural integrity and functionality in designed molecular assemblies [2].

A family of non-canonical amino acids (ncAAs) were synthesized using two complementary approaches: (1) Pd-catalyzed Negishi coupling of iodoalanine derivatives, and (2) Hofmann degradation of glycine or alanine to yield short-chain lysine homologues, followed by amidation or imidation. These newly synthesized ncAAs were incorporated into peptide sequences designed to form fiber-based hydrogels [3]. In sequences containing fluorescent naphthalimide moieties, both the gelation concentration decreased and gel strength improved. Additionally, aggregation-enhanced emission enabled detailed visualization of the fiber formation process through correlative fluorescence and atomic force microscopy imaging



These features make the resulting soft biomaterials promising candidates for applications in biosensing, real-time bioimaging, and 3D printing. They may also contribute to the development of drug delivery systems with sustained release profiles. Furthermore, the inclusion of redox-active groups within the peptide backbone is expected to facilitate electron transport, opening the door to future applications of these redox-active, nanostructured peptide materials in organic electronics.

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Embedding Relevance, Values and Identity in Chemistry Education

Marietjie Potgieter[a]

[a] Department of Chemistry, University of Pretoria, 0002 Pretoria, South Africa,

Keywords: Education for sustainability, responsible chemistry, ethical practice

As the urgency of global sustainability challenges intensifies, leading scholars in chemistry education have increasingly advocated for a fundamental reimagining of the teaching and learning of chemistry in recognition of chemistry's pivotal role in addressing these challenges at the molecular level [1]. A critical dimension of this transformation is the deliberate integration of ethics and values into chemistry education [2,3].

Chemistry, as a discipline, possesses immense dual-use potential: it can be harnessed to advance human well-being or exploited to cause significant harm. The accelerating pace of chemical innovation demands a parallel growth in ethical reflection and responsibility. Without this, we risk producing technically proficient chemists who are disconnected from the broader societal and environmental implications of their work. In response, the International Union of Pure and Applied Chemistry (IUPAC) has positioned "Responsible Chemistry" as a guiding value for the global chemistry community. This initiative was launched during the recent World Chemistry Congress in Kuala Lumpur, Malaysia [4]. A key outcome is the development of a set of eight Guiding Principles for the Responsible Practice of Chemistry, with accompanying educational resources, by the IUPAC Committee on Ethics, Diversity, Equity, and Inclusion [5]. The Guiding Principles provide a framework for transparent, responsible and ethical behaviour in all aspects of chemistry. It is designed to transform how chemistry is practiced, taught and perceived worldwide.

This presentation will explore recent IUPAC-led initiatives designed to embed responsibility, relevance, and ethical reflection at the heart of chemistry education and practice.

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Carbon-based nanocomposites for fourth-generation solar cells

Vincent Nyamori[a]

[a]School of Chemistry and Physics, University of KwaZulu-Natal, Westville Campus, Private Bag X54001, Durban, 4000, South Africa, Corresponding author e-mail address: nyamori@ukzn.ac.za

The increase in global energy demand has led to the extent that conventional energy sources, particularly fossil fuels, are facing a predicament due to their non-renewability. Additionally, they emit greenhouse gases that contribute to undesirable global warming and climate change. Thus, renewable and sustainable energy sources, particularly solar energy, which is abundant, clean, and cost-effective, are sought after. Currently, the first-generation (crystalline silicon) solar cells, which have relatively high power conversion efficiencies (PCEs), are the most commonly used. However, they are rigid, expensive, and require complex, high-energy fabrication procedures. Subsequently, second-generation (thin-film) solar cells, which are inexpensive and feature easy fabrication, emerged; nevertheless, they exhibit lower PCEs than their first-generation counterparts. Thus, the development of third- and fourth-generation solar cells, such as perovskite solar cells, dye-sensitised solar cells, and organic solar cells, has attracted significant research interests owing primarily to their facile fabrication procedures, low cost, lightweight, flexibility, easy scalability, low environmental impact, and ever-increasing PCE. However, their commercialisation has been set back by their relative instability and relatively lower PCEs. To circumvent these challenges, the recent emergence of novel materials, particularly carbon-based nanocomposites, is envisioned to help bridge the gap between fourth-generation solar cells and silicon solar cells. Carbon nanomaterials, due to their outstanding optoelectronic properties, excellent stability, nontoxicity, and low cost, have prompted much research effort. Their incorporation into fourth-generation solar cell components is envisaged to significantly increase the PCE, sustainability, environmental friendliness, and cost-effectiveness of devices.

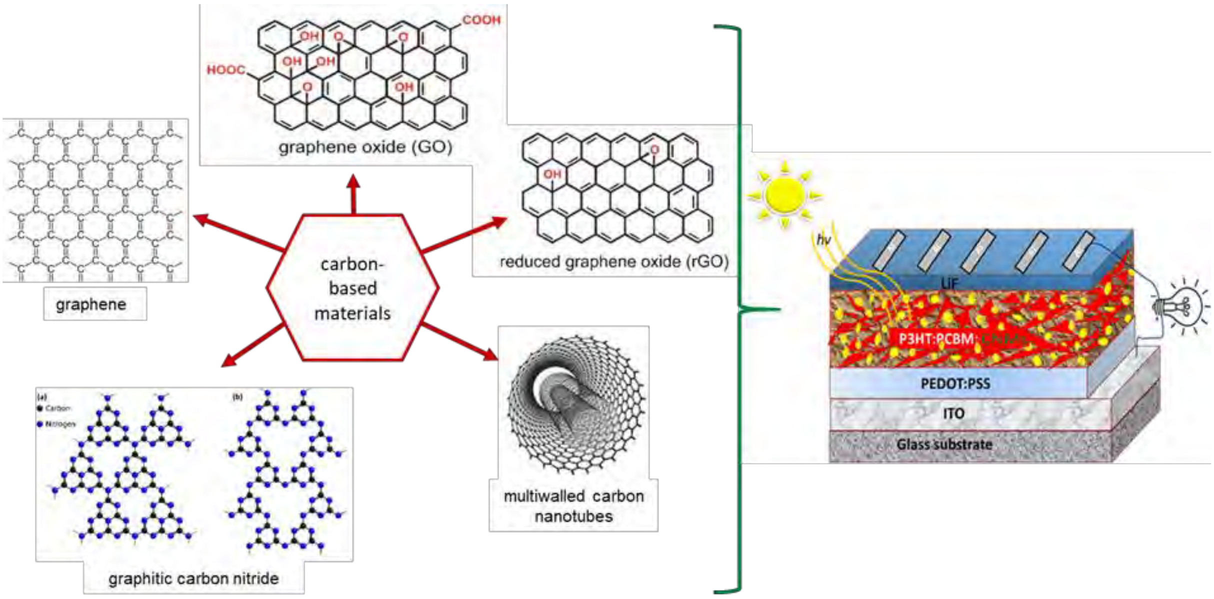

Figure 1: Selection of some carbon-based nanomaterials (CNMs) in fourth-generation solar cell fabrication.

Weighing Molecules to Treat and Diagnose Disease, from Viruses to Skin Swab

Perdita Barran[a]

[a]Michael Barber Centre for Collaborative Mass Spectrometry, Manchester Institute for Biotechnology, The University of Manchester, Manchester UK

Keywords: mass spectrometry, ion mobility mass spectrometry, Parkinson's Disease

Every year more than 30 million babies worldwide are screened for inborn metabolic disorders directly after birth with a heel prick assay that takes a tiny amount of blood to be analysed with a mass spectrometer[1]. In the UK every baby born is screened in this way. This program has improved the health and life chances of many babies. Other uses of mass spectrometry for health care include the analysis of therapeutics which increasingly are large and heterogenous with respect to mass. We have developed direct infusion methods and instruments to analyse monoclonal antibodies and adeno associated viruses.[2,3]

Our diagnostics research program uses mass spectrometry (MS) to find biomarkers for Parkinson's disease to enable diagnosis [4–7] . We do this from endogenous compounds obtained from skin swabs. In lab, we can determine if an individual has PD with >95% accuracy. Our unique research program has been initiated by Mrs. Joy Milne, a retired nurse from Perth who noticed a change in her husband's body odour 11 years before his clinical diagnosis of Parkinson's disease (PD). Joy noticed the same distinctive odour was associated with other PD sufferers and hence linked it to onset of the disease. Recently we demonstrated the equivalence of sebum to serum as a diagnostic biofluid[8] and shown that sebum can be stored at room temperature and still be useful. [9] Based on Joy's observation, with simple non-invasive sampling of skin from the upper back, we have developed a diagnostic platform that is able to classify PD from sebum samples with >95% accuracy. The focus of our work to date has been to detect and identify the compound(s) that encompass the unique odour of PD. We have now assessed the feasibility and quality of information provided by using sebum as a diagnostic biofluid via multiple mass spectrometry (MS) based analytical methods, and are now positioned to translate these methods, by incorporating clinical data to stratify PD diagnosis from prodromal to overt.

This talk will discuss our work in using mass spectrometry to analyse intact biomolecules, our methodological approach for biomarker discovery, recent findings and give a perspective on how non-invasive sampling and mass spectrometry could play a major role for prevention and effective treatment of disease.

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The Quest for Sustainable and Circular Battery Technologies - Operando X-ray Techniques probing Dynamic Processes in Batteries

Prof. Dr. Moniek Tromp[a]

[a] University of Groningen, Faculty of Science and Engineering, Zernike Institute for Advanced Materials, Materials Chemistry, Nijenborgh 3, 9747 AG Groningen, e-mail: Moniek.Tromp@rug.nl

Keywords: energy materials, batteries, performance, characterization

Batteries are of key importance in the energy transition, i.e. for mobility as well as for a temporary (intermediate) storage of excess energy (e.g. stabilise the grid). Li ion batteries are widely used in applications such as mobile phones and laptops, and will likely be key to future electromobility due to their low weight. Alternatively, more sustainable batteries are essential to enable the significant increase in demand as well as their differing applications and requirements (incl. local and grid storage), while reducing pressure on climate and environment.

Rational design of novel battery chemistries and technologies requires a detailed understanding of the charge, discharge and deactivation mechanisms, preferably quantitative and spatially resolved. X-ray techniques (spectroscopy and scattering) are characterisation techniques which provide detailed structural and electronic information on the material under investigation, in a time- and spatially resolved manner. These operando spectro-electroechemical investigations provide insights in the type, location and reversibility of the intermediates formed in and on electrodes and/or electrolytes as a function of state-of-charge and position in the battery. Obtained insights in cycling and deactiviation mechanisms for different battery types, i.e. Li-ion and Li-S, as well as more sustainable battery technologies like Ni-Fe and Fe-air, will be discussed and the strategy towards new sustainable batteries explained.

Multi-Purpose Nuclear Research Reactor

Neutron Beam Line Centre

Necsa Neutron
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PO Box 582
Pretoria 0001
South Africa

T +27 12 305 5038/5382
E useroffice@necsa.co.za
W www.necsa.co.za

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We're in your world

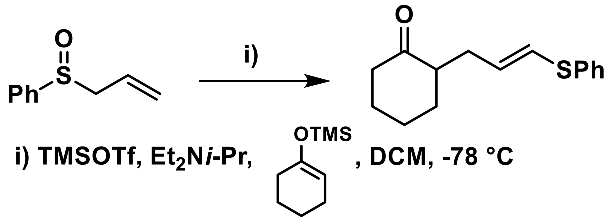
Organic Synthesis in South Africa: For Business or Pleasure?

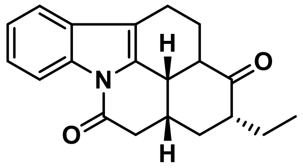
Roger Hunter[a]

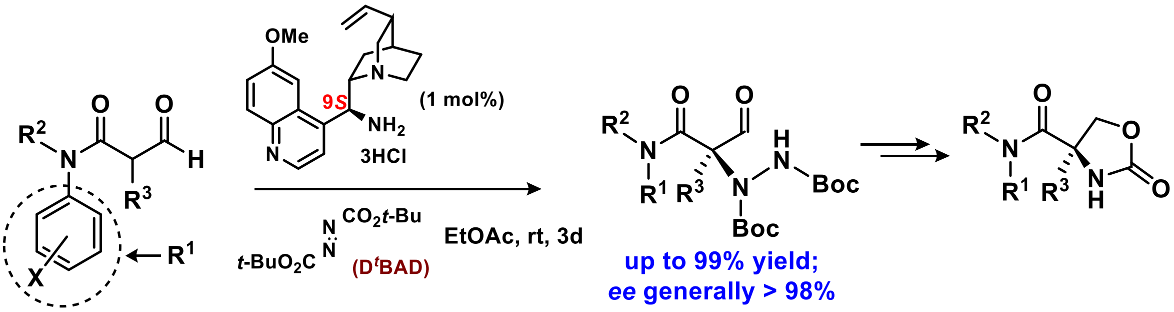
[a] Department of Chemistry, University of Cape Town, Rondebosch, 7701. Email: roger.hunter@uct.ac.za

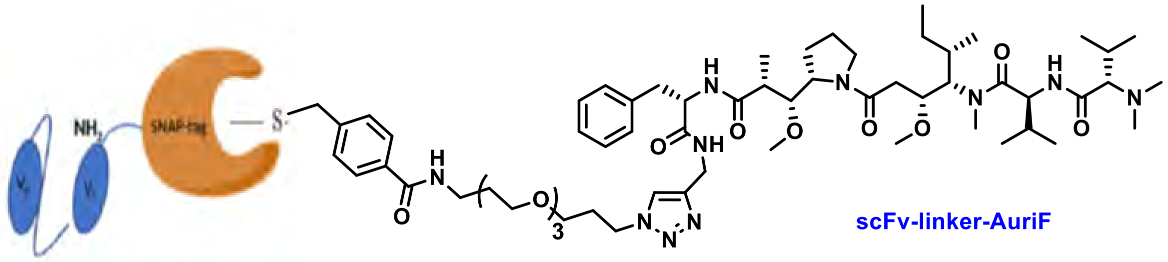
Keywords: organic synthesis, methodology, cancer

This lecture will describe my South African journey in organic synthesis, starting at Wits University in 1983 up to the present day at the University of Cape Town since 1989. It will present some of my methodological and synthesis contributions in organic chemistry for which I have received this award. It will also track how my research has had to adjust going from an intellectually hedonistic, end-in-itself era to the present-day, means-to-an-end business one, discussing the advantages and disadvantages of both paradigms. Some of my creations to be discussed in the lecture are highlighted in the Figure below.


A New Masked Michael Reaction[1]


Total Synthesis of (+)-Tacamonine[2]


Novel Organocatalysis α-Amination for Chiral, non-Racemic α-Tertiary Amine Motifs[3]


New scFv-Antibody-Drug-Conjugate for Cancer[4]

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Electrifying Chemistry for clean and affordable energy in Africa

Kenneth I. Ozoemena [a]

[a] DSI-NRF-Wits SARChI Chair in Materials Electrochemistry and Energy Technologies (MEET), Molecular sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa.
Email: kenneth.ozoemena@wits.ac.za

Keywords: Electrochemistry, lithium-ion batteries, zinc-based batteries, opportunity assessment

Electrochemistry has emerged as the 'saving grace' for the global quest for affordable and clean energy (UN 2030 Agenda for SDG #7) and clean transportation (electric vehicles). Electrochemical energy storage (EES), notably, the lithium-ion battery, is the third 'technology disruptor' (after digital camera and mobile phones). EES is the reason for the proliferation of portable electronics and mobile phones, the re-emergence and exponential growth in the development of electric vehicles (led by China), the rise in the off-grid electricity generation, especially the standalone 'Solar-Plus-Battery' pay-as-you-go electricity in rural Sub-Saharan Africa. EES is revolutionizing the Utility and transport industry, and transforming life, business and the global economy. It is obvious that without R&I efforts in EES, most critical aspects of modern living would be impossible. Africa is richly endowed with all the resources (human and raw minerals) to lead the world in EES. Unfortunately, the huge skills shortage in SET (science, engineering and technology), lack of the necessary R&I resources and infrastructure, and other reasons beyond the scope of this work have not allowed the continent to maximize its competitive advantage of beneficiating raw minerals and improving their economy. For example, there is no industry that manufactures lithium-ion batteries in Africa, and every battery-powered technology is imported. Unlike Africa, some Western countries have already set dates to ban petrol- and diesel-driven vehicles which will put more pressure on EES for electric vehicles, and default dumping of these rejected unclean vehicles in Africa. Another identified pressure on EES will be the rise in energy-thirsty AI-based technologies such as the ChatGPT. Over the years, our research group has been focusing on developing lithium-ion batteries [1,2].

In recent years, we have extended our R&I effort toward "beyond Lithium-ion battery" technologies, especially the "rechargeable zinc-air batteries (RZAB)" [3]. In this SACI Gold award presentation, I will provide situation analysis and opportunity assessment for Sub-Saharan Africa, and our R&I progress in developing lithium-ion batteries and zinc-based batteries.

[1] KI Ozoemena and CJ Jafta, "Production of a spinel cathode material", US Patent 9, 834, 854.
[2] KI Ozoemena and CJ Jafta, "Production of a layered lithium-manganese-Nickel-Cobalt oxide material", US Patent 10, 396, 357.
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The joy of research in separation science

Egmont R Rohwer [a]

[a] Department of Chemistry, University of Pretoria, Pretoria, South Africa; Email: Egmont.rohwer@up.ac.za.

Keywords: trace organic analysis, mass spectrometry, chromatography, interdisciplinary science

Both the research topics and the motivation behind a lifetime of research in the field of Chromatography and Mass Spectrometry will be discussed. A love for instrumental detail, together with a physical chemical approach to understanding and developing these demanding analytical techniques, gave rise to ideas that opened up novel methods for analyzing complex mixtures, mostly at trace quantitative levels.

Trace organic analysis always implies addressing improved selectivity to prevent signal overlap between the thousands of compounds found in the air, water, food and beverages, chemical industry, and the human body. Most often extraction of a more concentrated sample from the less informative matrix has to be performed off-line to improve sensitivity and to reduce bulk interferents like air, water, solids, and biopolymers. After further separation of the analytes with the best possible chromatographic techniques, the highly sensitive mass spectrometer has to be coupled in line for unique fingerprinting of individual compounds.

Examples will be given of how innovative (i) sample preparation, (ii) chromatographic, and (iii) mass spectrometric techniques were combined for tackling difficult analyses from environmental, aroma, geological, insect communication, industrial, and clinical samples. The research inevitably led to the challenge of interdisciplinary studies in order to plan experiments and extract relevant information from successful chemical analysis. Lack of funds often threatened the repair and replacement of our equipment and prevented deeper studies in a given field of expertise. We were lucky that our curiosity and love for wanting to make a real difference consistently led us to new collaborative projects, with new inspiring scientists, that helped provide funds for the survival of the expensive analytical laboratory. This approach even led to contributions in the trans-disciplinary fields of malaria control and off-grid rural African development [1].

The unusual reference to emotion in the title of this talk is intentional and meant to encourage academic scientists to nurture their personality-dependent passions and not to give up on their wildest research dreams despite the well-known pressures to over-specialize in order to obtain recognition, funds, and a regular stream of publications. The joy of discovery and dreaming of making a difference, addressing the Sustainable Development Goals, is the driver that kept the author going, even in very challenging times. I believe this is the only academic environment that is conducive to educating post-graduate students for their unknown tasks ahead.

[1] Preserving cultural diversity in rural Africa using renewable energy; Emil Roduner and Egmont Rohwer; Global Challenges. 2024, 8, 2300263 pp 1-7 DOI: 10.1002/gch2.202300263.

Molecular Precursor Strategies for Solid Solutions and High-Entropy Materials in Electrocatalysis

Malik Dilshad Khan[a]

[a] Department of Chemistry, University of Zululand, Private Bag X1001, KwaDlangezwa, 3886, South Africa.
Email: malikdilshad@hotmail.com

Keywords: Molecular precursors, solid solutions, colloidal synthesis

Controlling the properties of nanomaterials is traditionally achieved through size regulation, yet precise size control often requires complex synthetic routes, costly capping agents, and suffers from limited scalability. An alternative paradigm is to tune material properties through composition control, opening pathways toward solid solutions and medium to high-entropy materials with tailored functionality.

In this talk, I will present our approach of using molecular precursors as a versatile strategy to design and synthesize multicomponent nanomaterials. A key challenge in preparing solid solutions lies in balancing the relative reactivity of different precursors, as mismatched reactivity often leads to phase separation rather than homogeneous substitution. By systematically testing a range of precursor chemistries and synthetic conditions, we demonstrate the preparation of diverse cationic and anionic solid solutions, with compositionally tunable structures and properties. Extending this concept, we also explore medium to high-entropy materials derived from carefully selected precursor combinations, where configurational entropy further stabilizes complex solid solutions.

Electrochemical investigation highlights that compositionally tuned electrocatalysts show strong potential for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), where adjusting composition provides an effective pathway to optimize catalytic activity without relying solely on nanoscale size effects [1-4].

This composition-driven strategy illustrates a powerful, scalable approach to designing functional nanomaterials for energy conversion, offering new opportunities for sustainable electrocatalysis.

[1] Khan et al. *ACS Applied Energy Materials 3 (2), 1448-1460*.
[2] Malima et al. RSC advances 11 (49), 31002-31014.
[3] Malima et al. Scientific Reports 13 (1), 22179
[3] Shombe et al. RSC advances 12 (17), 10675-10685

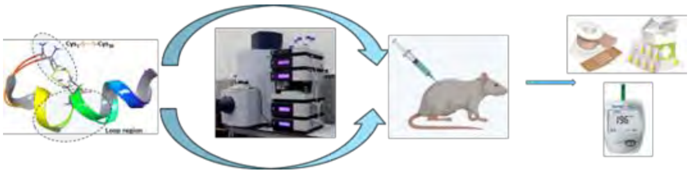
From Molecular Adventures to Wellness: Translating Peptidomimetics and Mass Spectrometry into Therapeutic and Diagnostic Innovations

Maya M. Makatini [a]

[a] Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, PO WITS, 2050, Johannesburg, South Africa Email: maya.makatini@wits.ac.za

Keywords: Peptidomimetics; Wound healing; Antimicrobial peptides; Diagnostics

Peptide-based research links molecular-level design to clinically relevant outcomes.



Our research focuses on developing stable peptidomimetics designed to inhibit or mimic key proteins in biological pathways. In the first part of the presentation, I will highlight three areas of progress: 1. Wound healing peptides targeting integrins, which significantly improved tissue repair in murine models.[1]. 2. Antitubercular peptides designed to interact with Mycobacterium tuberculosis caseinolytic protease, exhibiting both inhibitory and activating properties.[2] 3. Biocatalytic peptides mimicking fructose-1,6-bisphosphate aldolase, achieving good enantioselectivity (up to 93%)[3].

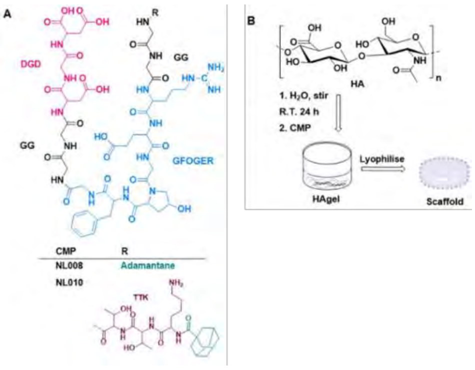


Figure 1. (A) Chemical structure of synthesized adamantane-based CMPs for wound healing and (B) graphical illustration of the formulation of the hyaluronic acid (HA) and CMP hydrogel (HAgel) and scaffold used for characterization. [1]

Our approach integrates medicinal chemistry-driven backbone and side-chain modifications to enhance protease resistance, membrane activity, and overall efficiency, supported by scalable solid-phase peptide synthesis. Structural characterization employs LC-MS, NMR (including ROESY), circular dichroism, and computational modelling. Notably, lipophilic conjugation strategies have improved antimicrobial and wound-healing efficacy, as demonstrated in recent publications.[1,2] The second part of the presentation focuses on mass spectrometry-based diagnostics, including early detection of diabetic nephropathy through amino acid ratios and peptide-based arsenic binding for point-of-care devices in mining health.

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[2] Cobongela, S. Z. Z.; Makatini, M. M.; May, B.; Njengele-Tetyana, Z.; Bambo, M. F.; Sibuyi, N. R. S. *Antibiotics* **2024**, *13* (2), 183.
[3] Peme, T.; Brady, D.; Shumbula, N. P.; Machumele, K.; Moloto, N.; Adams, T.; Makatini, M. *Catalysts* **2024**, *14* (11), 826.

Chemistry as an ideal central area for sustainability-related multidisciplinarity

Liliana Mammino [a]

[a] Faculty of Science, Engineering and Agriculture, University of Venda, University Road, Thohoyandou 0950, South Africa Email: sasdestria@yahoo.com

Keywords: education, disciplines, interdisciplinarity, interfaces

Multidisciplinarity is broadly acknowledged as a necessity for the pursuit of sustainability. On the other hand, the operational aspects of "how to go about it" are still largely to be identified or designed. Because of its nature as the science of substances, chemistry can interface with practically all the other disciplines, and the interfaces are capable of bringing constructive and novel contributions.

The presentation outlines individual interdisciplinary routes between pairs of disciplines, as well as the overall complex network of interactions that may result. The first considered ensemble of interactions regards the interactions between the different branches of chemistry. It is followed by the consideration of the ensemble of interactions between chemistry and the other disciplines, including humanities-pertaining ones. The ways in which three or more disciplines jointly contribute to the addressing of certain issues are analyzed through the consideration of concrete examples, with the analysis following patterns that are ready for presentation to students. For instance, chemistry contributes to the design of resilient and sustainable buildings through its role within materials sciences (where it interfaces with physics) and also through its role within geology (geochemistry). In terms of education, chemistry constitutes an ideal ground for the education to the use of language in science development and communication; this role entails interactions among chemistry concepts, language and philosophy, and builds two factors important for the pursuit of sustainability: conceptual understanding in chemistry and adequate language mastery.

The conclusions reiterate the essential function of multidisciplinarity and stress the importance of adequately incorporating attention to it into chemistry education, so that students develop into future specialists capable of constructively "talking to each other" across specialization areas and disciplines.

Pharmaceuticals as chemicals of emerging concern in East London major estuaries and seawater

Ronewa Netshithothole [a], and Lawrence M. Madikizela [b]

[a] Biodesign Institute Center for Environmental Health Engineering, Arizona State University, United States of America
[b] Institute of Nanotechnology and Water Sustainability, University of South Africa, Florida 1710, South Africa

Keywords: Pharmaceuticals, Chromatographic analysis, Environmental monitoring, Marine and coastal environment

Among chemicals of emerging concern, pharmaceuticals were extensively monitored in the South African environment (in the last decade), with most studies focusing their attention on river water and wastewater. This study focused on investigating the occurrence of ibuprofen, naproxen, sulfamethoxazole, trimethoprim, and efavirenz, which represent non-steroidal anti-inflammatory drugs, antibiotics, and antiretroviral drugs, along the East London coastline. The applied analytical method was based on solid-phase extraction of pharmaceuticals followed by a liquid chromatography-quadrupole time-of-flight mass spectrometry analysis. This analytical method proved to be sensitive, with method detection limits ranging from 0.16 to 9.44 ng/L. In terms of accuracy, the analytical method yielded recoveries ranging from 75 to 107%. Ibuprofen had concentrations reaching 90 ng/L in seawater. However, efavirenz and sulfamethoxazole were found to have high ecotoxicological risks toward aquatic organisms in river water. In addition, 57 other pharmaceuticals belonging to different therapeutic classes, including metabolites, were detected in various samples through non-target analysis. The results of this study showcase a long list of pharmaceuticals that could be considered for regular monitoring in the South African aquatic environment.

[1] Preserving cultural diversity in rural Africa using renewable energy; Emil Roduner and Egmont Rohwer; Global Challenges. 2024, 8, 2300263 pp 1-7 DOI: 10.1002/gch2.202300263.

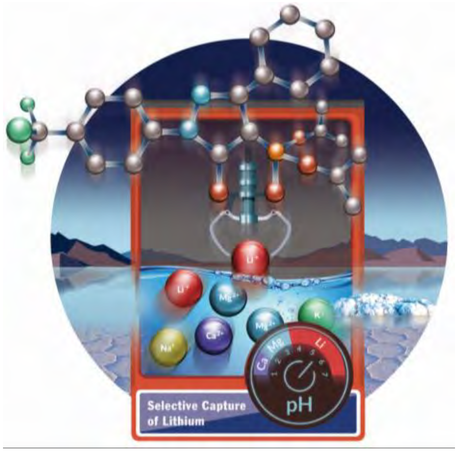
Molecularly Tuned 4-Phosphoryl Pyrazolones for Lithium Recovery and Selective Rare Earth Extraction

Jianfeng Zhang[a,b], *Marco Wenze*[a], *Felix Hennersdorf*[a], *and Jan J. Weigand*[a,c]

[a] Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden, German, E-mail: jan.weigand@tu-dresden.de. [b] Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China. [c] Department of Chemistry and Polymer Science, Stellenbosch University, Private Bag X1, Matieland, Stellenbosch 7602, South Africa

Keywords: lithium extraction, 4-phosphoryl pyrazolone, solvent extraction, rare earth elements, supramolecular complexation, pH-controlled selectivity

The sustainable recovery of lithium and related strategic metals is a key challenge in energy transition technologies. Herein, we present a structurally guided approach using 4-phosphoryl pyrazolone ligands in pH-controlled liquid-liquid extraction (LLE) systems. These ligands enable highly selective separation of lithium from coexisting alkali and alkaline earth elements such as Na^+, K^+, Mg^{2+}, and Ca^{2+}, achieving extraction efficiencies of up to 94% under optimized conditions. In-depth NMR, MS, and SC-XRD studies reveal the formation of di- and trinuclear lithium complexes that correlate with extraction performance. Co-ligand effects, especially from trioctylphosphine oxide (TOPO), were systematically evaluated to enhance metal-ligand interactions and tune selectivity. Beyond lithium, preliminary results demonstrate that structural modifications to the pyrazolone scaffold allow controlled interaction with rare earth elements (REEs), highlighting the potential of this ligand platform for broader separation applications. This work provides mechanistic and structural insight into alkali-REE separation and opens a pathway toward ligand-tailored, greener extraction systems.



Acknowledgment: We gratefully acknowledge financial support from the China Scholarship Council (CSC) and the Deutsche Forschungsgemeinschaft (DFG, WE 4621/5-1). This work was further supported by the CAS Key Laboratory of Green Process and Engineering and the Faculty of Chemistry and Food Chemistry at TU Dresden.

[1] Zhang, J.; Wenzel, M.; Yang, L.; Luckay, R. C.; Weigand, J. J. *Front. Chem. Eng.* **2023**, *5*, 1271045.
[2] Zhang, J.; Tanjedrew, N.; Wenzel, M.; Royla, P.; Du, H.; Kiatisevi, S.; Lindoy, L. F.; Weigand, J. J. *Angew. Chem. Int. Ed.* **2023**, *62*, e202216011.
[3] Zhang, J.; Wenzel, M.; Steup, J.; Schaper, G.; Hennersdorf, F.; Du, H.; Zheng, S.; Lindoy, L. F.; Weigand, J. J. *Chem. Eur. J.* **2022**, *28*, e2021036.

Atomistic Simulation of Atomic Level Processing Chemistries for Materials Deposition and Etch

Michael Nolan[a]

[a] Tyndall National Institute, University College Cork, Lee Maltings, Dyke Parade, Cork, Ireland
E-mail : michael.nolan@tyndall.ie

Atomic Level Processing (ALP), exemplified by Atomic Layer Deposition (ALD) and Atomic Layer Etching (ALE) is widely used in microelectronics and the semiconductor industry to deposit metals, oxide and nitride thin films as part of device fabrication in nano- or subnano-dimensions. Other technologies are embracing ALP for controlled materials processing in complex structures, including batteries and medical devices. The key advantages ALP are the uniformity, high conformality in deposition and etch, and precise thickness control at the atomic scale, which are difficult for physical or chemical vapor deposition methods at these length scales. The atomic scale understanding of ALP is vital and essential to design and optimize deposition processes, where density functional theory (DFT) calculations play an important role in providing detailed reaction mechanisms, theoretical screening of suitable precursors and estimated growth/etch-per-cycle (EPC/GPC), while allowing ALD chemistry of new processes to be explored. In this presentation I will discuss our work on a number of key areas in ALP. The first is the plasma enhanced deposition of Cobalt (Co) films. Co is of high interest in the semiconductor industry due to attractive electrical and physical properties and the possibility to replace Cu with Co as conductive contacts or interconnects in semiconductor devices. For PE-ALD of Co using CoCp2 and N/H-containing-plasma, we determined the state of the Co surface after a fill cycle followed by the reaction mechanism for the metal precursor pulse and for the first time, the plasma half-cycle on Co surfaces. We show the key role of nitrogen in activating the surface and removing Cp ligands, while H is also required to remove unwanted nitrogen, eliminate Cp and activate the surface, so only a plasma with both species will be effective in Co ALD. The next topic is the simulation of the self-limiting thermal atomic layer etch of high-k dielectrics, HfO_2, ZrO_2 and $HfZrO_4$ using fluorinated species and determining the impact of the phase and surface facet on the etch rate, which is important for polycrystalline nanoscale films. We find that both phase and surface facet have a strong impact on the etch rate with HF as the surface modifier and there are also differences between crystalline and amorphous films. We also explore how other fluorinated species could act as ALE reactants, assessing possible replacements for HF. Finally, I will discuss our methodological developments that we are applying to ALP chemistries. The first is a new kinetic Monte Carlo simulation tool that can model the deposition of metals on substrates, in particular tuning the metal-substrate interaction that allows for prediction of metal morphology. The second is development of machine learning potentials that can simulate long-time scale dynamics and activation barriers that are critical to all ALP processes. I will present results for trained ML potentials that are delivering new insights into metal morphology of interconnect metals on diffusion barriers.

Rational routes to porous carbons for sustainable energy applications

Robert Mokaya [a,b]

[a] School of Chemistry, University of Nottingham, University Park, Nottingham NG7 2RD, UK
[b] School of Mathematical and Physical Sciences, University of Sheffield, Dainton Building, Sheffield S3 7HF, UK
Email: r.mokaya@sheffield.ac.uk

The talk will explore the conversion of biomass and other waste carbonaceous matter to porous carbons with optimised properties for use in energy storage applications, and specifically the storage of CO_2, H_2 or methane. The talk will describe how study of a wide range of biomass and non-biomass precursors has enabled the predictable and targeted preparation of porous carbons with optimised properties for such sustainable energy applications.

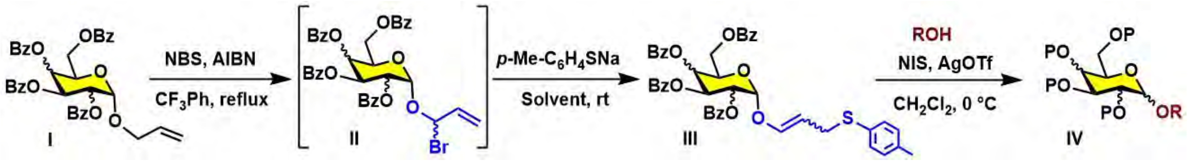
Remote Activation Route to Access Glycosyl Cation – The Case of 3-Thiocresyl-Prop-1-Enyl (TCP) Glycosides

Anupama Das, Deepak Kushwaha and N. Jayaraman [b]

[a] Department of Organic Chemistry, Indian Institute of Science, Bangalore 560 012, India; E-mail: jayaraman@iisc.ac.in

Keywords: Allyl glycosides, glycosylation, remote activation, thioether

Successful formation of oxocarbenium ion or glycosyl cation intermediate is a primary requirement in glycosylations, that lead to glycosides, in the form of oligo-, polysaccharides and myriads of glycoconjugates. Chemical glycosylations heavily rely on the substituent present at the anomeric carbon of a glycoside donor, which upon activation affords the reactive glycosyl cation intermediate. Reaction of this intermediate with a hydroxy functionality, completes the reaction and leads to the desired glycoside. A number of reactive functionalities at the anomeric carbon are developed over a period of time, in order to conduct the glycosylations, included with rigid stereochemical outcome of the resulting glycosides. Remote activation is an approach, where activation of a remotely located substituent induces inter- and intramolecular reactions, the result of which is the formation of the glycosyl cation intermediate, competent to afford a glycoside upon reaction with a glycosyl/aglycosyl acceptor. The basis of remote activation includes the presence of constituents in the aglycon portion of the glycoside, which upon activation encounters more than one covalent bond modifications, with concomitant glycosyl cation intermediate formation. We have developed 3-thiocresyl-prop-1-enyl (TCP) glycoside (**III**) as a suitable aglycon portion in a glycoside, amenable to remote electrophilic activation of the thiocresyl moiety. This activation initiates a cascade reaction, leading to the formation of glycosyl cation, which, in an one-pot reaction with glycosyl / aglycosyl acceptor, affords glycoside product (**IV**). TCP-glycosides are synthesized from allyl glycosides (**I**) in the steps of (i) allylic halogenation (**II**) and (ii) thiocresyl substitution occurring in an S_N2’-fashion. Glycosylations occur with a range of glycosyl / aglycosyl acceptors. The method is demonstrated with the synthesis of a number of target oligosaccharides, with the key glycosylations conducted using appropriate TCP-glycoside donors. Mechanistic details are followed to rationalize the reactions.
The presentation will exemplify the development of TCP-glycoside donors in glycosylations.



Scheme 1. Synthesis of TCP-glycoside **III** and glycosylations thereof to glycoside **IV**.

[1] Kushwaha, D.; Das, A.; Jayaraman, N. *Chem. Eur. J.*, 2025, **31**, e202500372 (1 of 7).

Humanity faces a bright future, and so Chemistry

Ehud Keinan [a]

[a] The Schulich Faculty of Chemistry, Technion-Israel Institute of Technology, Haifa 3200003, Israel;
Email: keinan@technion.ac.il

Humanity faces six global challenges:

1. Climate change and air quality
2. Sustainable energy
3. Dwindling raw materials
4. Water scarcity and safety
5. Food for everybody
6. Health problems

These problems are complex because they cannot be solved by known technologies, but future technologies will solve them. Because all six problems are primarily chemical issues, it is our responsibility and opportunity, as chemists, to meet these challenges. Everything is chemistry, and all sciences are chemistry because they all deal with matter, and all matter is made of atoms and molecules.

Humanity faces a bright future due to four reasons:

1. Knowledge explosion
2. Unpredictability of science
3. Evolution of network society
4. Human dignity and personal liberty

We live in artificial environments, eat genetically engineered food, wear synthetic and genetically modified fibers, and travel by fabricated devices. In other words, we live on products of human imagination and creativity, and since imagination and creativity have no limits, the effective area of planet Earth has no limits.

Therefore, the best ways to meet global challenges are:

1. Invest in education at all levels – encourage curiosity.
2. Invest in basic, high-risk, exploratory science.
3. Bolster human liberty, dignity, and democracy.
4. Encourage economic growth because only rich countries can afford good education, health, scientific innovation, and adaptation.

1. E. Keinan, Nurturing ‘wild horses’ in science is a universal goal: https://cen.acs.org/policy/research-funding/Opinion-Nurturing-wild-horses-science/103/i4
2. E. Keinan, Gloomy Forecast for the Prophets of Apocalypse and Bright Forecast for Chemists: https://doi.org/10.1002/anie.201209383
3. E. Keinan, Effective Area: https://doi.org/10.1080/23080477.2015.11665648

AI-Driven Innovations in Chemistry with Reaxys: Future Perspectives and Digital Transformation

Ivana Kotevic[a], *Marta Da Pian*[b], *Sherif Ghazy*[c]

Keywords: Reaxys, Predictive Retrosynthesis, Green Chemistry, Sustainability, Digital Transformation, Artificial Intelligence, Natural Language Query, Machine Learning

Structure Block/Scheme.
This session will provide an in-depth look into how AI is revolutionizing chemical research and discovery through the innovative capabilities of the Reaxys solution. Attendees will learn about recent advancements in AI-powered content extraction from patents and journals, including programmatic reaction and substance extraction driven by AI vision models. The session will also cover state-of-the-art predictive tools for retrosynthesis, synthetic accessibility, and green chemistry, showcasing how these technologies accelerate synthesis planning and promote sustainability. Additionally, the session will highlight enhancements in natural language queries, making data discovery more intuitive and relevant, as well as the seamless integration of Reaxys via APIs into existing workflows and digital ecosystems. By exploring real-world use cases, industry collaborations, and future AI developments, participants will gain insights into how Reaxys is supporting the digital transformation of chemistry and enabling researchers to tackle complex problems more efficiently and sustainably.

Target Audience: Chemistry Professors, Researchers, PhD Students, R&D Scientists, Data Scientists

Proposed Agenda Points/Session Plan:
1. Introduction & Overview of Reaxys AI Innovations
2. Content Expansion & Extraction Technologies
3. Predictive Tools for Synthesis & Green Chemistry
4. Enhancing Search via AI & Natural Language Processing
5. API Integration & Digital Transformation Use Cases
6. Future Roadmap & AI-Enabled Research Workflows
7. Q&A and Discussion

[a] Dr. Ivana Kotevic, VP Portfolio Product Management , Elsevier
[b] Dr. Marta Da Pian, Senior life sciences Account Manager– Europe South
[c] Dr. Sherif Ghazy, Life sciences Account Manager– Africa and Middle East

Reaxys

2025 roadmap update

Discover, innovate and develop with confidence

AI-powered search, expanded chemistry data and advanced technology help users optimize small molecule discovery and chemical R&D

The latest Reaxys developments

Launch of Reaxys AI Search

With Reaxys AI Search, users can now find chemistry literature using natural language queries. Built on Reaxys' trusted quality information, it quickly searches titles and abstracts from over 121 million documents, including 46 million patents. This tool makes it easier and more intuitive to discover relevant research, especially for complex or interdisciplinary topics. The early release of Reaxys AI Search marks the beginning of Reaxys' upcoming AI transformation.

Predictive Retrosynthesis enhancements

Reaxys offers multiple state-of-the-art predictive retrosynthesis models that accelerate research for synthetic, medicinal, computational and process chemistry teams. The latest improvements include:

- An updated model trained on recent Reaxys reaction data that provides a faster processing time and improves the diversity of synthesis routes
- Enhanced commercial substance integration with the largest library of commercial building blocks, now exceeding 150 million compounds, increasing the likelihood of successful predictions
- Automated adjustment of parameters to optimize route generation, reducing the instance of zero results
- A customizable retrosynthesis tool with models trained on Reaxys reactions and unpublished, proprietary ELN data to deliver predictions tailored to the specific chemical context of the company and accessible exclusively to the respective organization.

Content expansion and refinement

On top of regular content expansion, Reaxys has added 43 million make-on-demand analogues of screening compounds from Enamine, expanding to the existing 300 million commercial products. The integration provides chemists with unparalleled access to a diverse array of chemical compounds, facilitating the identification of novel drug targets, biomarkers and screening compounds.

Enhanced user experience

- New similarity sorting capabilities for both substances results and commercial products make it easy to find similar structures, supporting competitive intelligence and accelerating synthesis planning
- Updates on the user interface in compliance with the Web Content Accessibility Guidelines include the ability to resize text, view or hide additional content when hovering with a mouse or focusing with a keyboard, and bypass blocks to navigate more easily with screen readers or keyboard

Reaxys innovations coming in 2026

Reaxys continually invests in adding trusted quality chemistry data and advanced technology, so researchers have access to the most comprehensive and advanced resources.

Enhancement of Reaxys AI Search

Natural language search capability will be extended across the full Reaxys corpus. Research summaries and more updates will be added to support researchers across disciplines from materials science to drug discovery.

Accelerating content expansion

Reaxys will be using extractive AI technology in partnership with LG AI Research to improve the quality and quantity of extracted substances and reactions from patents and journals, helping enhance research productivity and innovation. The latest Vision Model technology will be used to enable faster access to the most relevant substance and reaction data through automated extraction.

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New technological advancements

- Launch of new Reaxys byproducts and impurities predictor for forward synthesis to support designing of safer and compliant reactions
- Update on features of IKTOS model like ignore stereochemistry (already released in April 2025), new cyclization templates and a new forward checker to improve the retrosynthesis predictions by broadening the scope, which enhances route diversity and reaction validity, respectively
- Improved synthesis planning with combined route predictions that integrate predicted and published reactions to suggest a broader range of viable, efficient and cost-effective options
- Launching the machine learning optimized reaction flat file to streamline data preparation, and to increase the number of reactions available for training and validating predictive models.

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Breaking barriers: Critical questions for the future of chemistry (Special session of SACI CDI)

Bice S. Martincigh[a] and Nikoletta B. Bathori[b]

[a]School of Agriculture and Science, University of KwaZulu-Natal, South Africa, [b]Department of Chemistry, Cape Peninsula University of Technology, South Africa.

Keywords: diversity, inclusivity, equity

Diversity and inclusion are widely recognised as essential for a thriving scientific community, yet the chemistry community continues to face challenges that deserve thoughtful reflection and open dialogue. This session will move beyond broad statements to consider some of the real barriers and opportunities shaping our field.

Through short contributions and a dynamic panel discussion, we will explore questions such as:
- What role does mentorship play in supporting students and early-career researchers from diverse backgrounds?
- How do we assess whether diversity initiatives are truly making a difference?
- How can cultural diversity in research groups and classrooms be recognised as a strength, while addressing the challenges it sometimes brings?

Rather than presenting fixed answers, this discussion aims to highlight different perspectives, share examples of effective practice, and identify possible directions for collective action.

The session is open and welcoming to everyone in the chemistry community, regardless of background, career stage, or experience with diversity initiatives. Progress depends on engagement from all voices, and we invite you to join this important conversation on building a stronger, more inclusive chemistry community.

This meeting also serves as a warm-up to the 2026 IUPAC Global Women’s Breakfast, creating momentum for continued dialogue and action on diversity and inclusion within chemistry at both national and international levels.

Innovating Chemistry: Designing Labs for Disability Inclusion

Ale Palermo [a]

[a] Royal Society of Chemistry, Burlington House, Piccadilly, London W1J 0BA

Keywords: diversity, inclusivity, equity

Ensuring that laboratory environments support the full participation of all scientists is increasingly recognized as a factor that directly influences research quality, productivity and innovation. This talk presents an evidence-informed case for integrating inclusive design and equitable practice into chemical laboratories and research settings. Rather than calling for large-scale infrastructural overhauls, we highlight practical, flexible approaches that apply the same creativity and problem-solving that drive chemical discovery to the design of our workspaces. Drawing on recent Royal Society of Chemistry findings, we will discuss how inclusion and diversity enhance scientific outcomes, and outline targeted recommendations for researchers, institutions, funders and policymakers. By treating inclusion as an initial design principle, and not as an afterthought consideration, we can reduce barriers that limit scientific potential and strengthen the resilience and excellence of the chemical sciences. This talk presents a roadmap for embedding these principles across the research ecosystem, demonstrating that designing for equity ultimately advances both scientific progress and has community-wide impact.

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Görkem Mergen [a] *and Sacha Devillers* [b]

[a]Görkem Mergen, PhD, Customer Success Manager, CAS - gmergen@acs-i.org
[b]Sacha Devillers, Sales Director of EMEA, CAS - sdevillers@acs-i.org

In this session, we will explore how CAS SciFinder® can be a valuable tool for identifying new career opportunities, preparing for job interviews, and connecting with potential mentors who can support you throughout your Ph.D. or postdoctoral journey.

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Chemistry and Quantum Science
(Special session : IUPAC Year of Quantum Science)

Andrew Forbes [a]

[a] School of Physics, University of the Witwatersrand, Johannesburg, South Africa

Keywords: quantum science; chemistry

To celebrate the UNESCO year of Quantum Science, the SACI 2025 Convention will have a special session dedicated to revealing how Quantum Science can play a role in Chemistry. This session has been sponsored by the South African Quantum Science Technology Initiative

This will take the form of a Plenary lecture, talks and a panel discussion. The Plenary Lecture will be given by Prof Greg Scholes, Princeton University, USA. The discussion will focus on the intersection of Quantum Science and Chemistry, and how chemists can play a role in the Quantum Sciences

The target audience for the event are chemists interested in learning about how quantum science can be used in chemistry
The panel session with be chaired by Prof Andrew Forbes (Physics, Wits) and the panel members are Prof Cornie van Sittert (Chemistry, NWU), Prof Tjaart Kruger (Physics, UP), Prof Greg Scholes (Princeton University, USA) and Prof Thomas Konrad (Physics, UKZN).

Two short talks will also be given by Prof Tjaart Kruger, and Prof Thomas Konrad as examples of how their areas of expertise on quantum science can be used in the chemical sciences.

Manipulating individual light-harvesting complexes with light

Tjaart P. J. Krüger [a]

[a] Department of Physics, University of Pretoria, Hatfield, 0083, South Africa, tjaart.kruger@up.ac.za

Keywords: single-molecule spectroscopy, gold nanoparticles, plasmonics, photosynthesis, light harvesting

The absorption and emission of light by a molecule are beautiful examples of quantum electrodynamics. In nature, they constitute immensely important single-photon events where quantum mechanics dictates the allowed transitions, lifetimes, and spectra. Photosynthesis is a prime example, starting with a single-photon absorption event, while fluorescence is often used as a sensitive reporter of the function, dynamics, and interactions of photosynthetic protein complexes. In this presentation, I will firstly show how metallic nanoparticles can be effectively used to significantly modify the photophysical rates of a nearby fluorescing molecule. Specifically, I will demonstrate that the fluorescence of individual light-harvesting complexes of plants can be enhanced by two orders of magnitude when coupled to chemically synthesised gold nanorods [1], showing an inexpensive platform to construct efficient hybrid light-harvesting devices. Secondly, I will demonstrate how the interaction between two individual light-harvesting protein complexes in cyanobacteria can be controlled with light using our homebuilt single-molecule spectroscopy setup [2, 3], a method that enabled us to discover and characterise an important docking mechanism. I will also show how we can obtain considerable insight into the underlying structural and energetic landscape of these complexes using quantum-chemical modelling [4].

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[2] Gwizdala, M., Berera, R., Kirilovsky, D., van Grondelle, R., Krüger, T.P.J. *J. Am. Chem. Soc.* 2016, **138**:11616-11622.
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[4] Cupellini, L., Gwizdala, M., Krüger, T.P.J., *J. Phys. Chem. Lett.* 2024, **15**:9746–9756.

Chemistry and quantum science

Thomas Conrad

[1] Kyeyune, F; Botha, J.L.; van Heerden, B; Maly, P; van Grondelle, R.; Diale, M; Krüger, T.P.J. *Nanoscale*, 2019, **11**:15139-15146.
[2] Gwizdala, M., Berera, R., Kirilovsky, D., van Grondelle, R., Krüger, T.P.J. *J. Am. Chem. Soc.* 2016, **138**:11616-11622.
[3] Gwizdala, M., Botha, J.L., Wilson, A., Kirilovsky, D., van Grondelle, R., Krüger, T.P.J. *J. Phys. Chem. Lett.* 2018, **9**:2426-2432.
[4] Cupellini, L., Gwizdala, M., Krüger, T.P.J., *J. Phys. Chem. Lett.* 2024, **15**:9746−9756.

Shaping the Future of Education in Analytical Chemistry: A Discussion

Megan Matthews[a],

[a] Department of Chemistry and Polymer Science, Stellenbosch University, Merriman Avenue, Stellenbosch, 7602, South Africa, E-mail: mmatthews@sun.ac.za.

Keywords: analytical chemistry, education, curriculum

Analytical chemistry is a cornerstone of scientific research and industry, underpinning advancements in fields such as environmental science, pharmaceuticals, forensics, food safety and materials science. As new technologies emerge and the demand for interdisciplinary skills grows, the landscape of education in analytical chemistry is rapidly changing.

Curriculum research [1] highlights a strong emphasis on standardization, calibration and instrumental methods such as UV–Vis spectroscopy, HPLC, and GC, alongside data handling and error analysis. While these priorities reflect international perspectives, they raise important questions about how analytical chemistry education in South Africa aligns with global expectations and local needs. These results also raise a critical tension in curriculum design: should we modernise to reflect emerging techniques and technologies or preserve long-standing core content that still underpins much of analytical practice? [2] While methods like UV-Vis and IR spectroscopy and chromatography remain central in both teaching and industry, their dominance may risk crowding out newer, interdisciplinary tools such as hyphenated techniques, real-time sensors or data science applications in analysis. Yet, abandoning the fundamentals too quickly may leave students without the conceptual grounding needed to innovate responsibly.

This panel discussion will explore current challenges, the changing requirements of modern teaching methods and future directions in analytical chemistry education. The aim of the discussion is to bring together educators and emerging scientists to explore how best to equip the next generation with the skills needed to tackle complex, real-world problems.

[1] Kovarik, ML; Galarreta, BC; Mahon, PJ; McCurry, DA; Gerdon, AE; Collier, SM. et al. *J Chem Educ*, 2022, **99**, 2317–26
[2] Fung, FM; Widyantoro, C; Li, SFY. *Anal Chem* 2024, **96**, 6863–9


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Development of a novel instrument for long-term measurements of OH reactivity

Midhun George[a], *Thomas D. Luke*[a], *Ambili. V. Babu*[a], *Lisa K. Whalley*[a,b], *Dwayne E. Heard*[a], *Mark A. Blitz*[a,b], *Thomas Wynn*[c] *and Daniel Stone*[a]

[a] School of Chemistry, University of Leeds, Leeds, LS2 9JT, UK, E-mail: M.George@leeds.ac.uk
[b] National Centre for Atmospheric Science (NCAS), University of Leeds, Leeds, LS2 9JT, UK
[c] School of Geography Earth and Environmental Sciences, University of Birmingham, Birmingham, B15 2TT, UK

Keywords: air quality, OH reactivity, UV absorption spectroscopy, field measurements

Improving air quality is a key challenge in achieving a sustainable future. Effective mitigation strategies for air pollution and climate change require accurate knowledge of both atmospheric trace gas concentrations and the chemical processes that govern their transformation. The primary sink for many trace species such as methane (CH_4), volatile organic compounds (VOCs), and nitrogen oxides (NO_x = NO + NO_2) is reaction with the hydroxyl radical (OH). These reactions drive the formation of secondary pollutants like ozone (O_3) and secondary organic aerosols (SOAs). Understanding the behavior of OH in the atmosphere is therefore essential to determining the lifetimes of trace gases and the pathways leading to secondary pollutant formation.

Although it is not feasible to measure all OH-reactive species directly, their collective impact on atmospheric chemistry can be assessed through measurements of OH reactivity (k_{OH}). OH reactivity represents the total pseudo-first-order loss rate of OH, defined as $k_{\mathrm{OH}} = \sum_{\mathrm{i}} k_{\mathrm{OH+X_i}}[\mathrm{X_i}]$, where $k_{\mathrm{OH+X_i}}$ is the rate coefficient for reaction of OH with species X_i.

Several techniques have been successfully used in the field to measure k_{OH} [1-4], but continuous long-term observations remain challenging, particularly in high-NO_x environments [5]. Here, we present the development of a novel instrument for long-term k_{OH} measurement, based on laser flash photolysis combined with time-resolved broadband UV absorption spectroscopy. The instrument is designed for long-term operation across a wide range of atmospheric conditions and achieves a limit of detection (LOD) of ~1.5 s^{-1} in its field configuration. We describe the instrument's design, performance characterization, intercomparison with a laser-induced fluorescence (LIF) instrument, and preliminary results from long-term deployment at the Birmingham Air Quality Supersite.

[1] Kovacs and Brune, *J. Atmos. Chem.*, 39, 105–122, 2001.
[2] Sadanaga *et al.*, *Rev. Sci. Instrum.*, 75, 2648, 2004.
[3] Sinha *et al.*, *Atmos. Chem. Phys.*, 8, 2213–2227, 2008.
[4] Stone *et al.*, *Atmos. Meas. Tech.*, 9, 2827–2844, 2016.
[5] Fuchs *et al.*, *Atmos. Meas. Tech.*, 10, 4023–4053, 2017.

Quantification and treatment of problematic odour-causing compounds in drinking water within Magalies Water Treatment systems and interrelated catchments

Phindile Mahlangu[a], *Maria Mashigo*[a], *and Letlhogonolo Mabena*[a]

[a] The Department of Chemistry, Arcadia Campus, Pretoria, 0001, South Africa, E-mail: phindilem@magaliewater.co.za.

Keywords: Ozone-infused nanobubbles, removal efficacy, metabolites, pre- and advanced treatment

Introduction

Source water impoundments, including lakes, rivers, dams, and groundwater aquifers, contain metabolites that can cause undesirable taste and odour characters, ultimately impacting the quality of treated water. Geosmin (GSM), 2-Methylisoborneol (MIB), and ammonia (NH_3) present significant challenges for contemporary water treatment processes due to their unpleasant aesthetic attributes and the ease with which consumers can detect them. The widely utilized technologies for their removal include Powdered or Granular Activated Carbon, Ozone, Chlorine Dioxide, and Filtration. These methods are limited by their high initial capital investment costs, increased waste contribution, and limited adsorptive capacity, making them economically impractical for eliminating odor-causing compounds in semiurban, financially constrained regions, necessitating cost-effective pre-treatment modalities.

Materials and Methods

Raw water samples were collected from the Pienaars River Catchment over two months period, between December and January, and were preserved until analysis. The concentrations of GSM and MIB were quantified using Gas Chromatography Mass Spectrometry (GC-MS), coupled with a Purge and Trap (P&T) method, while NH_3 was measured using an automated Discrete Gallery Analyzer. Ozone-infused nanobubbles (OINBs) were introduced into untreated source water before the application of conventional treatment methods. The average OINB concentration in the water was recorded at 0.8 mg/L of ozone, administered at a 10% factor of the process flow.

Results and Discussion

The study revealed that the source water is characterized by a significant concentration of NH_3, ranging from 0.5 to 55 mg/L, while the concentrations of Geosmin and 2-MIB were found to vary between 0.5 and 150 ng/L, which were significantly above their odor threshold concentrations. The findings indicated a commendable removal efficacy for GSM and 2MIB at 33.3% and 40.65%, respectively, while the removal efficacy for NH_3 was moderate, at 10.56%. Oxidation emerged as the primary removal mechanism for all contaminants, particularly through advanced oxidation processes (AOPs). The generation of OINBs by the Moleaer generator ensured their stability in water, which was crucial for their effectiveness. When combined with conventional treatment methods, OINBs enhance overall removal efficacy, which could be particularly beneficial during warmer seasons when water sources are heavily contaminated due to evaporation and contaminants' preconcentration.

Conclusion

The Nanobubbles (NBs) technology provides a cost-effective and sustainable bioremediation solution that can be executed with little to no infrastructure alterations, while ensuring zero chemical usage and minimal waste generation. The recent discovery is particularly compelling, as it not only embodies a futuristic approach but also aligns seamlessly with the Sustainable Development Goals (SDGs) framework.

Assessment of selected Potential Toxic Elements and risk associated during Seasonal variation at Hennops River, South Africa

Ramasehle Z Moswane[a, b *], *Nehemiah Mukwevho*[a,b], *Napo Ntsasa*[a,b], *Andile Mkhohlakali*[a], *Luke Chimuka*[b], *Happy Mabowa*[a], *Lebohang Mokwena*[a], *James Tshilongo*[a], *Mokgehle R Letsoalo*[a]

[a]Analytical Chemistry Division, Mintek, Private Bag X3015, Randburg 2125, Johannesburg, South Africa
[b]School of Chemistry, University of the Witwatersrand, Private Bag 3, WITS, 2050, South Africa
ramsehlem@mintek.co.za; Tel.: +27 11 709 4094

Keywords: water pollution, carcinogenic and non-carcinogenic risk, degree of contaminants (DC), pollution indices

Population growth and industrialization are among the key contributors to the pollution of freshwater ecosystems and including rivers. Chemical intrusion in the environmental water presents substantial ecological risks, often obstructing the accessibility of safe water for human populations. This study quantified the amount of potentially toxic elements in the river stream during seasonal variation to assess the pollution index and potential health risks. Among the potentially toxic elements evaluated (Fe, Mn, Zn, Ni, Mo, V, Co, Cu), the highest concentration in water was recorded for Fe, ranging from 2180-29600 µg/L during the wet season and from 513-1723 µg/L in dry seasons. The lowest concentrations of potentially toxic elements were detected for Cu, ranging between 20.0-28.2 µg/L during the dry season and were undetectable in the wet season. The quantitative pollution indicators assessed in water quality highlighted values ranging from significant pollution to extreme contamination of pollution load index, geo-accumulation, enrichment, and contamination factors, particularly during the dry season, indicating heavy pollution. Statistical analysis revealed that strong correlation coefficient between Fe-Mn, with $r = 0.94$ and $r = 0.70$ in both respective wet and dry seasons, with a p-value of 0.063, indicating a significant correlation, suggesting possible same sources. The assessed health risk evaluation, with a hazard index exceeding 1 for both adults and children, indicates a probable exposure to non-carcinogenic effects. The risk of cancer assessment is markedly elevated, averaging 0.176 for adults and an alarming 0.258 for children, indicating a severe cancer risk even during the wet season, which exhibited low levels of some selected potentially toxic elements. The study emphasises the pressing demand for rigorous pollution control regulations focusing on remediation initiatives, and effective enforcement of regulations to minimize potentially toxic elements pollution.

Investigating the occurrence of pharmaceutical residues in urban estuarine water using grab and passive sampling approaches with UHPLC Q-Orbitrap MS analysis – A case of Durban Marina, South Africa

Sabetha Mapetla[a], *Nondumiso Mofokeng*[ab], *Heidi Richards*[a], *Brent Newman*[c], *Kuria Ndungu*[d], *and Luke Chimuka*[a]

[a]Molecular Sciences Institute, School of Chemistry, University of Witwatersrand, Private Bag X3, Johannesburg, 2050, South Africa, E-mail: 604060@students.wits.ac.za. [b] Mpact Innovation, Research & Development, Devon Valley Road, Stellenbosch, 7600, South Africa. [c] Coastal Systems and Earth Observation Research Group, Council for Scientific and Industrial Research (CSIR), P.O. Box 59081, Umbilo, Durban, 4075, South Africa. [d] Environmental Chemistry and Technology, Norwegian Institute for Water Research (NIVA), Økernveien 94, NO-0579 Oslo, Norway

Keywords: emerging contaminants, high resolution mass spectrometry, passive sampling, pharmaceutical residues, solid-phase extraction, urban estuaries

Monitoring pharmaceuticals in marine environments is challenging due to their dynamic nature and the ultra-trace concentrations at which these contaminants occur. This study investigates the occurrence of nine pharmaceuticals from various therapeutic classes in Durban Harbour, an urban estuarine system in South Africa. Two sampling techniques—passive sampling using Chemcatcher and grab sampling with solid-phase extraction (SPE)—were evaluated for their effectiveness in detecting and quantifying these compounds. Analysis using ultra-high performance liquid chromatography coupled with high-resolution mass spectrometry (UHPLC-HRMS) achieved detection and quantification limits of 0.15–2.18 ng L^{-1} and 0.50–7.27 ng L^{-1}, respectively. Chemcatcher was calibrated for five compounds, including three for which sampling rates in seawater (0.34–0.42 L day^{-1}) are reported here for the first time. Chemcatcher exhibited a consistent pharmaceutical detection frequency of 88.89%, while SPE detections ranged from 55.56% to 77.78%. Lopinavir and trimethoprim were undetected in several SPE samples but were consistently present in all Chemcatcher extracts. Chemcatcher also yielded higher total concentrations (824.81–2574.52 ng L^{-1}) compared to SPE (36.07–221.66 ng L^{-1}). To our knowledge, this is the first report of dexamethasone, lopinavir, metformin and methocarbamol in South African marine waters. These findings highlight the limitations of grab sampling in dynamic estuarine systems and support the integration of passive sampling into long-term marine water quality monitoring programs.

Understanding the Environmental Impact of SCCPs: Detection in Consumer Products, Landfill Leachate, and Sediments from Gauteng

Vhodaho Nevondo[a], *Okechukwu Jonathan Okonkwo*[a]

[a] Department of Environmental, Water and Earth Sciences, Faculty of Science, Tshwane University of Technology, 175 Nelson Mandela Drive, Pretoria Central, 0001, South Africa, E-mail: vhodahonevondo@gmail.com

Keywords: CPs, SCCPs, Landfill, Leachate, Sediment

Chlorinated paraffins (CPs) are commonly used as additives in various consumer products, such as polyvinyl chloride (PVC) materials, mining conveyor belts, paints, sealants, adhesives, and flame retardants. Due to their widespread use, CPs have been detected in multiple environmental media. Among the different types of CPs, short-chain chlorinated paraffins (SCCPs) have attracted significant global attention because of their toxicity, environmental persistence, and ability to undergo long-range atmospheric transport. In recognition of these hazardous properties, SCCPs were added to the Stockholm Convention on Persistent Organic Pollutants (POPs) in May 2017. At the eighth Conference of the Parties (COP-8), it was agreed that SCCPs with carbon chain lengths from C10 to C13 and chlorine content exceeding 48% by weight must be phased out. Furthermore, the SCCP content in other CP formulations was restricted to less than 1% by weight, meaning any CP mixture containing 1% or more SCCPs is now classified as a POP. The toxicological effects of SCCPs are considered more significant than that of MCCPs and LCCPs. Human exposure to SCCPs primarily occurs through inhalation of contaminated dust and dietary intake. Consequently, SCCPs have been detected in the blood, breast milk, placenta, hair, and nails. The toxicity of SCCPs has been linked to a range of harmful effects, including lethality, liver damage, developmental and reproductive toxicity, cancer, endocrine and metabolic disruption, and immune system modulation in both humans and animals.

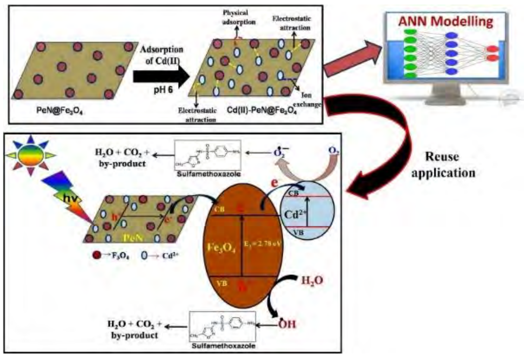
In most developing countries, general waste, including SCCP-containing consumer products waste is usually disposed of in municipal landfill or dump sites. When SCCP-containing consumer products reach the end of their useful life, they are frequently discarded in landfills, where they can release contaminants into the surrounding environment through leaching. This study investigates the presence and concentrations of SCCPs (51.5 and 55.5% chlorine content) in selected consumer products, landfill leachate, and sediment samples from Gauteng Province, South Africa. SCCPs were detected across all matrices, with concentrations in consumer products ranging from 12.03–439.58 ng/g (51.5% Cl) to 87.77–344 ng/g (55.5% Cl). Sediment and leachate concentrations varied between sites, with higher levels observed in Goudkoppies compared to Hatherly. These findings highlight the pervasive presence of SCCPs and underscore the need for stricter environmental monitoring and management to mitigate their potential risks. Therefore, consumer products waste need to be monitored as relevant potential source of SCCPs worldwide, even where the national industry strictly follows the restriction of such chemicals.

Magnetically-derived pecan nutshells for the removal of cadmium: artificial neural network modelling and photodegradation of sulfamethoxazole.

Akinshola O. Akinola, Eswaran Prabakaran, Krishna Govender, and Kriveshini Pillay

[a] Department of Chemical Sciences, University of Johannesburg, Doornfontein Campus, Johannesburg, South Africa. E-mail: akinsholaakinola@gmail.com

Keywords: Cadmium ions, wastewater, artificial neural network, photocatalyst, sulfamethoxazole



Cadmium has been labelled as a heavy metal hazardous to plants, animals and humans because, upon exposure, it can cause major health problems such as lung cancer, renal damage, and bone degeneration[2] [3]. This study explored the use of a nanocomposite, $PeN@Fe_3O_4$, made from pecan nutshells modified with magnetic Fe_3O_4, for removing cadmium ions (Cd^{2+}) from wastewater. The magnetic $PeN@Fe_3O_4$ was synthesised from pecan shells and analysed using techniques such as FTIR (Fourier Transform infrared spectroscopy), SEM (Scanning electron microscope), EDX (Energy dispersive x-ray), TEM (Transmission electron microscope), XRD (X-ray diffraction spectroscopy) and BET (Brunauer–Emmett–Teller) analyses. It exhibited a pore volume of 0.3888 cm^3/g and a surface area of 64.81 m^2/g, which is approximately 33 times larger than that of the unmodified PeN (1.953 m^2/g).

This material showed a high adsorption capacity of 63.29 mg/g and achieved over 90% removal efficiency in tests with actual wastewater samples. Kinetic analysis indicated that Cd^{2+}adsorption follows a pseudo-second-order model, while the Freundlich isotherm best describes the equilibrium state. The Cd^{2+}-loaded $PeN@Fe_3O_4$ was also reused as a photocatalyst after multiple cycles of adsorption-desorption to break down the antibiotic sulfamethoxazole, achieving 99% efficiency. To optimise the adsorption process, an artificial neural network (ANN) model was developed using a Python multilayer perceptron regressor, which accurately predicted both the removed amount and the removal efficiency of $Cd^{2+}$with a mean absolute error of 0.1091, a mean squared error of 0.0440, and an R^2 value of 0.9998. The results suggest that $PeN@Fe_3O_4$ is a promising material for environmental cleanup. Its capacity to remove Cd^{2+} and degrade organic pollutants in a closed-loop system offers an eco-friendly wastewater treatment method. The ANN model serves as a useful tool for forecasting and enhancing adsorption performance, thereby maximising contaminant removal and aiding in producing clean water. This approach reduces secondary pollution from spent adsorbents, supporting sustainable remediation strategies.

1 UNICEF & WHO, *Progress on household drinking water, sanitation and hygiene 2000–2017: Special focus on inequalities. In New York and Geneva: UNICEF*, 2019.
2 N. A. Ibrahim, F. H. H. Abdellatif, M. S. Hasanin and M. M. Abdellatif, *J. Clean. Prod.*, 2022, **332**, 130021.
3 Y. Liu, T. Xiao, R. B. Perkins, J. Zhu, Z. Zhu, Y. Xiong and Z. Ning, *J. Geochemical Explor.*, 2017, **176**, 42–49.

Bioprospecting Phytochemicals from banana plant wastes mediating Green Synthesis of Metallic Nanoparticles

Jonathan M. Mukanya[a], *and Rosalyn Klein*[a]

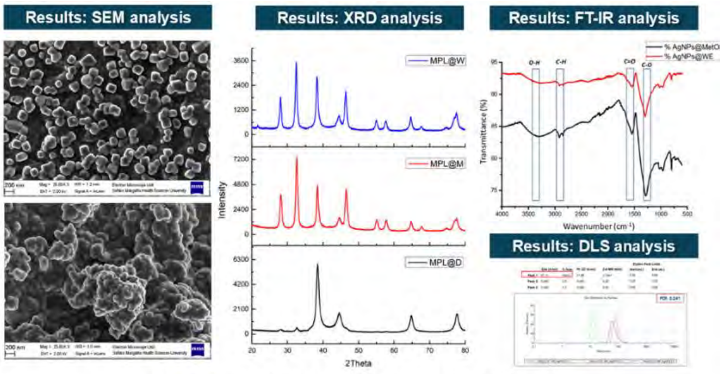
[a] Department of Chemistry,Rhodes University, Makhanda 6140, South Africa

Keywords: green synthesis, metallic nanoparticles, phytochemicals

The integration of nanotechnology and natural product research presents a promising frontier for developing sustainable biomedical applications. While metallic nanoparticles (NPs) are recognized for their antimicrobial and therapeutic potential, conventional physical and chemical synthesis routes often face challenges such as toxicity, scalability, and biosafety. Biological synthesis methods, particularly plant-mediated "green synthesis," provide eco-friendly and cost-effective alternatives by exploiting phytochemicals as reducing and stabilizing agents.

This study aims to elucidate the phytochemical basis of green synthesis by focusing on two Musa species (*Musa paradisiaca* and *Musa sapientum*). Plant extracts and fractions were systematically screened and used for the synthesis of silver nanoparticles (AgNPs).

Phytochemical characterization was performed using LC-MS/MS, FTIR, and UV-Vis spectroscopy, while nanoparticles were analyzed by UV-Vis, FTIR, XRD, DLS, SEM, and TEM to assess their physicochemical properties. Additionally, the biological activities of phytochemicals and corresponding nanoparticles, including antimicrobial and antioxidant assays, were evaluated to establish functional relevance.



Characterizations of silver nanoparticles synthesized plant extracts

The outcomes highlight the potential of Musa-derived metabolites in producing stable, bioactive AgNPs, while contributing to a deeper understanding of metabolite–nanoparticle formation mechanisms. This approach advances bioprospecting for safer nanomaterials and supports the translation of green nanotechnology into biomedical applications.

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Household Microwave-Assisted Green Synthesis of Biocompatible Gold Nanostructures Using *Aloe Africana* for Biomedical Applications

Thabang C. Lebepe [a, b]

[a] Department of Chemical Science, University of Johannesburg, Johannesburg, 2028, South Africa, E-mail: calvyn.tl@gmail.com.
[b] Centre for Nanomaterials Sciences Research, University of Johannesburg, Johannesburg, 2028, South Africa

Keywords: Nanoclusters; Green synthesis; Aloe Africana; Biomedical; Antibacterial

Gold nanoclusters (AuNCs) are increasingly valued for their unique optical and biological properties [1]. However, traditional synthetic methods often rely on toxic and costly chemicals, which limit their potential in biomedical applications [2]. This study presents a simple, microwave-assisted green synthesis method for producing blue-green fluorescent AuNCs and photothermal active gold nanoparticles (AuNPs) using Aloe Africana leaf extract.

We systematically evaluated the effects of various factors on the properties of AuNCs, including gold salt concentration (ranging from 0.001 to 0.05 M), pH (from 3 to 12), and the gold-to-extract volume ratio (1:2, 1:1, and 2:1). The optimal conditions for synthesizing AuNCs were determined to be 0.01 M gold salt concentration, pH 12, and a 1:2 ratio, resulting in AuNCs with an average size of 1.98 ± 0.98 nm, an emission peak at 450 nm, and a quantum yield of 2.17%. For AuNPs, the optimal conditions were 0.005 M gold salt, pH 3, and a 1:2 ratio, producing nanoparticles with an average size of 14.26 ± 4.05 nm and generating heat up to 44.5 °C when irradiated with an 808 nm laser. Fourier-transform infrared spectroscopy (FTIR) analysis confirmed the presence of phenolic and carbonyl groups, which play key roles in reducing and stabilising the nanoparticles. Both AuNCs and AuNPs exhibited excellent photostability at 37 °C for 48 h.

Additionally, Aloe-AuNCs demonstrated a molecular binding constant of 1.47×10^{-2} with DPPH, indicating their potential as nanocarriers. Antimicrobial studies showed a dose-dependent inhibition of both S. aureus and E. coli. Cytotoxicity tests on THP-1 cells indicated up to 90% cell viability, with RNA integrity comparable to untreated controls. These results highlight Aloe Africana as a promising green source for synthesising stable and biocompatible gold materials, which have potential applications in bioimaging, photothermal therapy, drug delivery, and antimicrobial treatments.

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Harnessing raw and the magnetized fly ash as low cost adsorbents for the removal of pharmaceuticals from wastewater: Isotherms and kinetics

Maqqira Bavuyile[a], Prof Precious Mahlambi[a]

[a] Department of Chemistry, University of KwaZulu-Natal, Private Bag X01, Scottsville, Pietermaritzburg, 3209l, South Africa, E-mail: 220010172@stu.ukzn.ac.za.

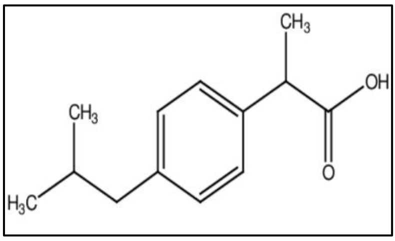
Keywords: adsorption, wastewater treatment plants, effluents, low-cost adsorbent, circular economy

Pharmaceutical compounds are increasingly recognized as emerging contaminants in aquatic environments due to their widespread use and incomplete removal by conventional wastewater treatment processes. These substances, frequently detected in surface waters and effluents, pose significant ecological and health concerns even at trace concentrations. While traditional adsorbents such as activated carbon and zeolites are effective, their high cost, limited regeneration potential, and reduced efficiency at low concentrations highlight the need for more sustainable and accessible alternatives.

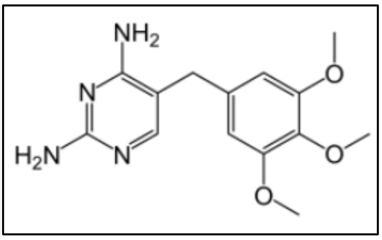
This study investigates the potential of using raw fly ash, an abundant by-product of coal combustion, as a low-cost and eco-friendly adsorbent for pharmaceutical removal from wastewater. To enhance its adsorption capacity, the fly ash was further modified through acid treatment, which alters its surface characteristics and porosity. Both raw and acid-modified fly ash were characterized using FTIR, PXRD, SEM, TEM, BET, and TGA analyses. These techniques confirmed notable changes in surface area, pore structure, and functional groups due to acid modification, which are hypothesized to contribute to improved adsorptive performance.

Batch adsorption experiments were conducted to evaluate the removal of three representative pharmaceuticals (trimethoprim, dolutegravir, and ibuprofen). Liquid chromatography-mass spectrometry (LC-MS) was used for precise quantification of contaminants at trace levels. Adsorption isotherms and kinetic models revealed that acid-modified fly ash exhibited superior removal efficiency and faster adsorption rates compared to raw fly ash, owing to its enhanced surface reactivity. These findings suggest that acid-modified fly ash offers a promising, scalable, and circular solution for pharmaceutical remediation, repurposing industrial waste into a valuable material for water purification.

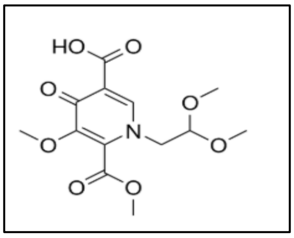
Structure Block/Scheme.



Ibuprofen



Trimethoprim



Dolutegravir

Investigating the Pharmacological Potential of Ferrocenylbenzimidazole Complexes as Antimalarial and Anticancer Agents

Remofilwe Manye[a], *Siyabonga Ngubane*[b] *and Prinessa Chellan*[a]

[a] Department of Chemistry and Polymer Science, Stellenbosch University, Office Suite 2039, Stellenbosch, 7600, South Africa, E-mail: rmanye@sun.ac.za.
[b]Department of Chemistry, University of Cape Town, North Lane, Rondebosch, 7700, South Africa

Keywords: ferrocene, benzimidazole, antimalarial, anticancer

The search for new malaria and cancer treatments remains crucial, given the persistent threat of malaria and the rising resistance of *Plasmodium falciparum* to current drugs, as well as cancer's scourge on humanity.[1], [2] One promising strategy is hybridization, which combines active pharmacophores to enhance efficacy, introduce multiple mechanisms of action, and reduce the risk of resistance.[3], [4], [5]

This study reports the synthesis and characterisation of seven novel ferrocenylbenzimidazole derivatives, each bearing a different substituent (R group) at the **C5** position of the benzimidazole core (
Figure ***1***). Two of the derivatives were designed as Schiff base ligands and subsequently coordinated to Ir(III), Rh(III), and Ru(II), yielding six heterobimetallic complexes; three cationic, and three neutral.

Physicochemical analyses confirmed that all complexes were sufficiently stable and soluble in aqueous environments under physiologically relevant conditions. Electrochemical investigations revealed that the redox behaviour of the compounds was influenced by the ligand environment, solution pH, and the presence of a secondary metal centre.

Biological evaluation against *Plasmodium falciparum* (NF54 strain) showed that the complexes displayed moderate antiplasmodial activity, with a heterobimetallic ruthenium complex exhibiting the highest potency. Preliminary anticancer screening against three breast cancer cell lines (MCF-7, T-47D, and MDA-MB-231) indicated modest cytotoxicity, with selective activity observed against MCF-7 cells, suggesting potential for further development.

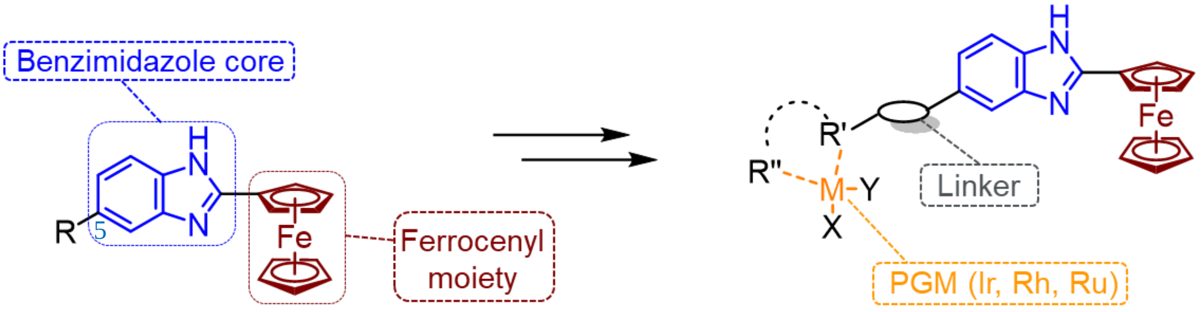


Figure 1: General schematic representation of the studied complexes.

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A Modular Continuous Flow Synthesis of Primaquine Diphosphate an Anti-malarial Drug

Faith M. Akwi[a] *and Paul Watts*[a]

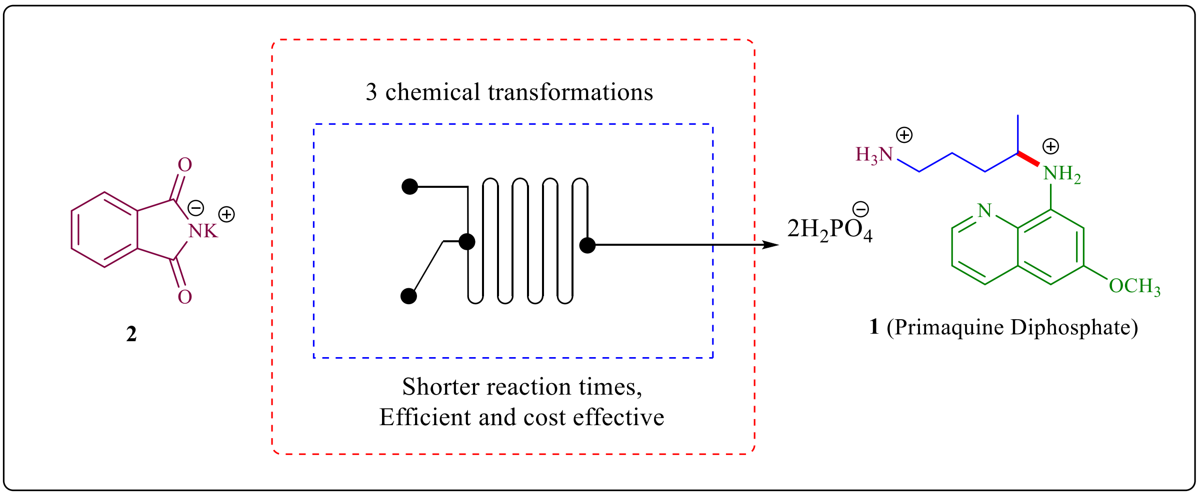
[a] Department of Chemistry, Nelson Mandela University, University Way, Port Elizabeth, 6031, South Africa., E-mail: s211206296@mandela.ac.za

Keywords: continuous flow synthesis, anti-malarial, active pharmaceutical intermediates

Malaria is one of the world's most infectious diseases. It is present in over 80 countries with the most affected population being children under 5 years of age, pregnant women and HIV-AIDS patients.[1] According to the WHO's 2019 World Malaria Report, there were 229 million cases and an estimated 409,000 deaths worldwide while in 2018, 228 million cases and 411,000 deaths were recorded. The African region was reported to have accounted for 94% of all global cases and deaths; 67% of deaths worldwide were of children under the age of 5 years.[2] It is therefore paramount that access and availability to potent anti-malarials be improved especially in low developing economies. This can potentially be achieved through local drug manufacture and capacity development.

As part of our vision towards pioneering regional drug manufacture on the African continent, it is one of our objectives to establish efficient synthetic routes towards numerous active pharmaceutical intermediates using both batch and most especially enabling technologies such as continuous flow processing. As such, we herein report for the first time the continuous flow synthesis of Primaquine Diphosphate **1**, an antihypnozoite 8-aminoquinoline compound reported to be extremely active against exo-erythrocytic stages of *P. vivax* and *P. ovale*, primary exo-erythrocytic stages of *P. falciparum* and gametocytes.[3]

The target molecule **1** was furnished from readily available potassium phthalimide **2** *via* three chemical transformations; phase transfer catalyzed *n*-alkylation, reductive amination and phthalimido deprotection all in good yields and in shorter reaction times compared to the batch processes disclosed in literature.[4]



2

1 (Primaquine Diphosphate)

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Eco-friendly extraction of saponins from the leaves of *Musa paradisiaca* and their formulation into micelles for the co-encapsulation of antimalarial drugs

Pathy Lokole[a,b], *Vincent Smith*[a], *Christian Nkanga*[b], *Roderick Walker*[c]

[a] Department of Chemistry, Rhodes University, Makhanda, 6140, Eastern Cape, South Africa, E-mail: g24l7497@campus.ru.ac.cd. [b]*Centre de Recherche en Nanotechnologies Appliquées aux Produits Naturels* (CReNAPN), Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmaceutical Sciences, University of Kinshasa, B.P. 212, Kinshasa XI, Democratic Republic of the Congo. [c]Division of Pharmaceutics, Faculty of Pharmacy, Rhodes University, Makhanda, 6140, Eastern Cape, South Africa

Keywords: Saponins, saponin-based micelles, *Musa paradisiaca*, malaria, mechanochemistry

Saponins are a significant class of phytochemicals known for their diverse properties. They have been used in drug delivery, cosmeceutical and vaccine formulation applications [1]. In a preliminary work, we have extracted saponins from five different plant species, explored their ability to self-assemble into biocompatible saponin-based micelles (SBM) and investigated their entrapment efficacy using a hydrophobic molecule—isoniazid-grafted-phthalocyanine (Pc-INH). The results showed less *in vitro* hemolysis of SBM (10%) compared to crude saponins (150%); Moreover, DLS and TEM showed nano-sized SBM's particles, which presented encapsulation efficiency of 55%, the drug loading capacity of 2.3% and a pH-dependent release over time of Pc-INH [2]. Taken together, these results place SBM as a potential drug delivery system with a high potential to improve the aqueous solubility of hydrophobic drugs.

Despite their self-assembly potential, saponins are usually extracted by a traditional method, which is time-consuming (two weeks) and involves the use of several hazardous organic solvents. Herein, we report an optimised eco-friendly extraction method of saponins from *M. paradisiaca* leaves—mechanochemical-assisted extraction" (MCAE). We have used the planetary ball mill submitted to different speeds (200, 400 and 600 rpm) and times (20, 40 and 60 min), water and chemical auxiliaries (malic acid, $NaHCO_3$ and NaOH) which improve the extraction of saponins thanks to the mechanical action of the planetary ball mill [3]. The saponins extracted from the optimum conditions (malic acid while 60 min at 400 rpm) were analysed and identified using Q-TOF-LC-MS, confronting the potential of MCAE to be used as a green, time-saving and efficient method for the extraction of saponins.

The well-known self-assembly method of saponins into SBM was applied to address the issue of the low bioavailability of Artemether and Lumefantrine used in the first line of the treatment of non-complicated malaria, a deadly infectious disease. Several plant-based nanoparticles are extensively used in the co-encapsulation of antimalarials [4]; However, SBM is potentially one of the easiest, biocompatible and cost-effective drug delivery systems as demonstrated in this project, where we have co-encapsulated Artemether and Lumefantrine and well characterised by different solid-state techniques—SEM, TEM, FTIR, DSC, TGA and PXRD. Further liquid-state characterisations are ongoing to establish the encapsulation efficiency and drug loading capacity from optimised formulations using a validated HPLC method and DLS.

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The photodynamic antimicrobial and anticancer activity properties of porphyrin, corrole, chlorin and N-confused porphyrin complexes

[a] *John Mack, Balaji Babu, Rodah C. Soy, Somila Dingiswayo, Kristen P. Burgess, Godfred E. Sebiawu, Mahlatse Ledwaba, Kaisano G. Tauyakhale, Vicky L. Kembou, Pertunia R. Macigane, Shakhola E. Sekeleme, Zine Gwaji, Nolwazi Zitha and Tebello Nyokong*

[a] Institute for Nanotechnology Innovation, Rhodes University, Makhanda 6140, South Africa, E-mail: j.mack@ru.ac.za.

Keywords: porphyrins, corroles, chlorins, N-confused porphyrins, PDT, PACT, photophysics

Over the last five years, considerable progress has been made with a rational structural modification approach [1,2] to prepare porphyrin analogues with significantly red-shifted and intensified Q bands that are suitable for use as photosensitizer dyes in photodynamic therapy [2-13]. When corrole, chlorin and N-confused porphyrins (NCPs) are formed by introducing a pyrrole-pyrrole bond, a reduced peripheral pyrrole bond and a confused pyrrole nitrogen atom, respectively, there is a significant red shift of the lowest energy Q band into the phototherapeutic window (620−850 nm). The introduction of thienyl *meso*-substituents further enhances the red shift of the Q band due to a narrowing of the HOMO−LUMO gap [2,5], leads to higher Φ_Δ values, and facilitates the preparation of gold and silver nanoparticle conjugates [3,4], while *meso*-vanillin rings can enhance the lipophilicity properties of the complexes [9,10]. Octabromination of the porphyrin ligand also results in a significant red shift and intensification of the porphyrin Q band due to ligand saddling, and also significantly enhances the Φ_Δ values [13].

Novel corroles [3,4], chlorins [5-9], NCPs [9-12] and octabromoporphyrins [13] have been prepared along with their Sn(IV), Ga(III) and/or P(V) complexes so that aggregation effects can be hindered by *trans*-axial ligation. When series of structurally analogous complexes have been prepared with the same *meso*-aryl groups [7-9,12], significantly lower IC_{50} values have been obtained for the corrole, chlorin and NCP analogues during *in vitro* photocytotoxicity studies against MCF-7 breast cancer cells relative to the parent porphyrin. Interestingly, high log reduction values have been observed with chlorin and NCPs complexes against both Gram-(+) *S. aureus* and Gram-(−) *E. coli* strains despite the absence of positively charged moieties on the ligand, which are normally required to obtain significant PACT activity against Gram-(−) bacteria. Further progress made with similar studies that are currently in progress will also be described.

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Polymeric encapsulation of artemisinin-ferrocene hybrids as a route towards enhanced antimalarial delivery

Stacey Roman[a], Prinessa Chellan[b] and Rueben Pfukwa[a]

[a] Department of Chemistry and Polymer Science, Stellenbosch University, Private Bag X1, Matieland, 7602, South Africa
E-mail: sroman@sun.ac.za

Keywords: malaria, artemisinin, ferrocene, micelles

The rise in malaria-related mortality, particularly in sub-Saharan Africa, is largely driven by resistance to existing antimalarial drugs. Artemisinin-based combination therapy (ACT) remains a frontline treatment.[1] However, many antimalarial agents suffer from toxicity and poor physicochemical properties, such as low water solubility and stability, which limit their effectiveness. Controlled and targeted drug delivery is gaining interest for enhancing therapeutic outcomes.[2] Nanoparticles have emerged as promising carriers, offering improved solubility and stability, enhanced membrane transport, prolonged circulation time, and potentially increased drug safety and efficacy.[3,4]

Three artemisinin-containing ferrocene complexes were successfully synthesized and characterized using a range of analytical techniques. These complexes demonstrated potent antimalarial activity against the *P. falciparum* NF54 strain, showing comparable efficacy to their parent compounds. The polymer-based drug delivery system was developed using the amphiphilic block copolymer poly(ethylene glycol)-*block*-poly(lactic acid) (PEG-*b*-PLA), which self-assembles in aqueous environments to form nanosized micelles capable of encapsulating hydrophobic drugs. The process of self-assembly as well as encapsulation was monitored and the micelles with sizes ranging from 18-35 nm were analyzed using various techniques. The encapsulated drugs demonstrated promising antimalarial activity and showed potential for enhancing the stability and solubility of the active compounds.

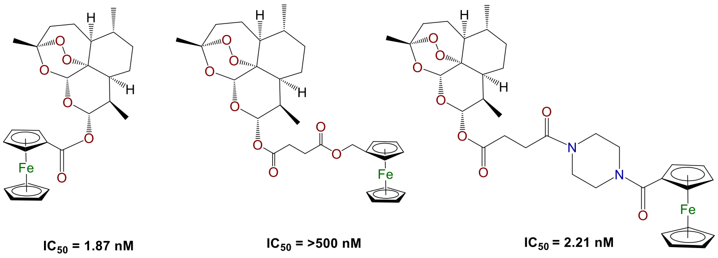

Figure 2: Chemical structures of artemisinin-ferrocene hybrid compounds designed for antimalarial therapy.

Acknowledgements

This research project was funded by the National Research Fund (NRF) and the Future Leaders – African Independent Research (FLAIR) Fellowship.

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Synthesis and evaluation of waste-derived metal-organic frameworks for hydrogen storage

Henrietta Langmi[a], Keaoleboga Mosupi[a], Nokubongwa Dlamini[a], Christophe Ndamyabera[a], Mike Masukume[b] and Nicholas Musyoka[c]

[a]Department of Chemistry, University of Pretoria, Private Bag X20, Hatfield, 0028, South Africa, E-mail: henrietta.langmi@up.ac.za. [b]Centre for Nanostructures and Advanced Materials (CeNAM), Chemicals cluster, Council for Scientific and Industrial Research (CSIR), Meiring Naude Road, Brummeria, Pretoria, 0001, South Africa. [c]Nottingham Ningbo China Beacons of Excellence Research and Innovation Institute, University of Nottingham Ningbo China, Ningbo 315100, PR China

Keywords: metal-organic frameworks, waste valorization, sustainable synthesis, hydrogen storage

Metal-organic frameworks (MOFs) are a class of crystalline materials formed through the coordination of metal ions or clusters with organic ligands. Due to their unique characteristics such as exceptionally high surface areas, modifiable pore sizes, large internal volumes, tunable chemical functionalities, MOFs have gained widespread attention for their potential in numerous fields. These include gas storage and separation, catalysis, sensing, drug delivery, environmental remediation, among others. Compared to traditional porous materials like zeolites and carbon-based structures, MOFs offer superior versatility and performance. However, their widespread application is limited by challenges in synthesis, including the use of toxic solvents, elevated temperatures, lengthy reaction times, and expensive starting materials. In response, there is growing interest in more environmentally friendly and cost-effective methods for MOF production. This presentation focuses on our research on sustainable MOF synthesis using waste-derived resources. Specifically, we explore the use of discarded aluminium-based materials and acid mine drainage as metal sources, along with polyethylene terephthalate (PET) bottles as a source of organic linkers. The structural and functional properties of the resulting MOFs, along with their hydrogen storage performance will be discussed. This work showcases a greener route to MOF fabrication that supports scalable production for broader practical use.

Green Synthesis of Cerium/Carbon-Modified NiS Nanoparticles Using *Sutherlandia frutescens* for Photocatalytic Dye Degradation

Carol Langa[a], *Nonhlangabezo Mabuba*[b] *and Nomso Hintsho-Mbita*[a]

[a] Department of Chemistry, Faculty of Science and Agriculture, University of Limpopo, Sovenga, Polokwane 0727, South Africa, E-mail: caroldmk.langa@gmail.com [b]Department of Chemical Sciences, University of Johannesburg, Doornfontein Johannesburg 2028, South Africa

Keywords: Nis nanoparticles, *Sutherlandia frutescens*, photocatalysis, Congo red dye

The increasing presence of synthetic dyes in wastewater highlights the urgent need for multifunctional, eco-friendly photocatalysts. In this study, nickel sulfide (NiS) nanoparticles were synthesized using *Sutherlandia frutescens* plant extract, offering a green and sustainable route to nanomaterial production. NiS samples were calcined at varying temperatures (uncalcined, 300 °C, 500 °C, and 700 °C) and characterized using XRD, FTIR, UV-Vis, TGA, BET, and SEM. SEM revealed grain-like morphologies and increased aggregation at higher temperatures, hence the crystallite sizes increased from 15 to 28 nm. Photocatalytic tests against Congo Red dye under UV light showed the sample calcined at 300 °C exhibited the highest degradation efficiency (70%), with hole species (h^+) identified as the dominant reactive species. To further enhance the photocatalytic performance of the NiS nanoparticles, cerium ions (Ce^{3+}/Ce^{4+}) and carbon spheres were introduced as modifying agents. Cerium was selected for its redox versatility, which may facilitate improved charge separation, while carbon spheres were incorporated to increase surface area and provide additional active sites. Preliminary results suggested that the combined incorporation of cerium ions and carbon spheres into the NiS matrix shows promising potential for enhancing photocatalytic degradation efficiency through synergistic effects. These findings emphasise the potential of green-synthesized NiS nanocomposites as efficient and environmentally friendly materials for wastewater treatment and applications.

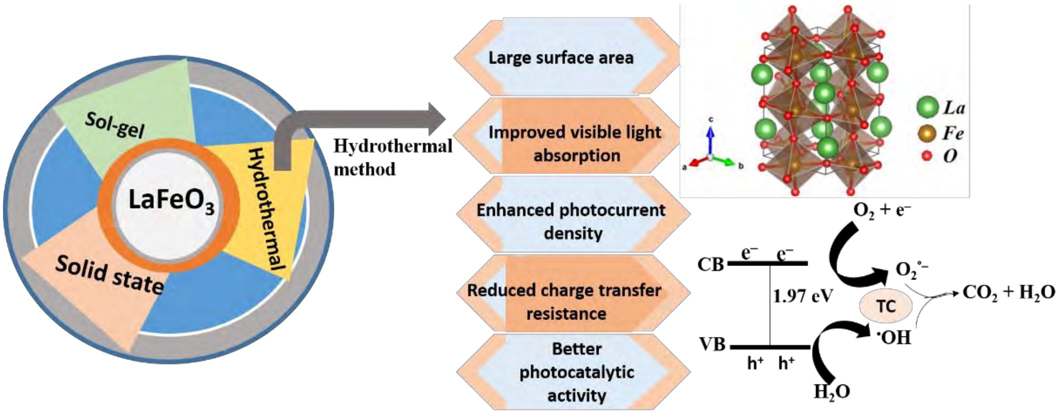
Synthesis route matters: Interrogating the structural, morphological, optical, surface, photoelectrochemical and photocatalytic properties of lanthanum ferrite perovskite

Oluchi V. Nkwachukwu[a,b,*], *Gugulethu P. Ndima*[a,b], *Omotayo A. Arotiba*[a,b,*]

[a]Department of Chemical Sciences, University of Johannesburg, Doornfontein, 2028, South Africa
[b]Centre for Nanomaterials Science Research, University of Johannesburg, South Africa, Email: oarotiba@uj.ac.za

Keywords: Sol-gel synthesis; solid state synthesis; hydrothermal synthesis; lanthanum ferrite; photocatalytic degradation

The catalytic properties of $LaFeO_3$ particles rely on their stoichiometric composition and microstructure, which are affected by the synthesis routes [1,2]. In this study, the influence of sol-gel, solid state, and hydrothermal synthesis methods on the properties and photocatalytic application of lanthanum ferrite ($LaFeO_3$, LFO) perovskite material is reported. The LFO from each synthesis route was characterised with XRD, XPS, FTIR, Raman spectroscopy, FESEM, HRTEM, and Brunauer-Emmeth-Teller (BET) analysis. The hydrothermal LFO possessed the most improved light-harvesting capability and charge recombination suppression as shown by UV-vis-DRS and photoluminescence studies. The hydrothermal LFO generated the highest photocurrent density, suggesting the highest current mobility. Lower charge transfer resistance and improved photodegradation reaction kinetic were observed at the hydrothermal LFO photoanode [3]. The extent of tetracycline mineralization, measured by total organic carbon (TOC) analysis for LFO from sol-gel, solid state, and hydrothermal routes, was 62.5, 55.0, and 77.5% respectively. LCMS provided information on the degradation and fragmentation patterns of the photocatalytic degradation process. This study shows that the synthesis route can affect the overall performance of $LaFeO_3$ perovskite oxide.



TC = Tetracycline

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Synthesis and evaluation of dosimetrics features of silica nanoparticles derived from *Musa paradisiaca* pseudostem

Galilée G. Byamungu[a,c], *Makaiko L. Chithambo*[a], *Christian I. Nkanga*[c], *Bertha Chithambo*[a], *Rui W.M. Krause*[a], *Rosalyn Klein*[a]

[a]Department of Chemistry, Faculty of Sciences, Rhodes University, PO Box 94, Grahamstown 6140, Eastern Cape, South Africa. [b]Department of Physics and Electronics, Rhodes University, PO BOX 94, Grahamstown, 6140, South Africa
[c]Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmaceutical Sciences, University of Kinshasa, B.P. 212, Kinshasa XI, Democratic Republic of the Congo.

Keywords: *Musa paradisiaca*, silica nanoparticles (SiNPs), thermoluminescence, radiation dosimetry

The use of high dose radiation technologies is currently crucial in many fields of human technical activity [1]. However, human unwanted exposure to radiation either during routine radiation work or due to accidental causes, may lead to numerous health hazards depending on the radiation type and the absorbed dose [2,3]. In this context, the development of agricultural wastes thermoluminescent materials appears to be a promising pathway for the manufacture of ecofriendly and cost-effective substrates for radiation dosimetry useful in the prevention of radiation risks to human health. Plantain (*Musa paradisiaca*) pseudo-stem (waste) consisting of about 76.72% of the plant mass could be a source of SiNPs, a thermolunescent material [4,5]. The goal of this research project is to explore the potential of *Musa paradisiaca* pseudostem-derived silica nanoparticles in radiation dosimetry.

Sol gel method was used to synthesize SiNPs and thermoluminescence measurements were made using RISØ TL/OSL Reader model DA-20 on samples irradiated using a ^{90}Sr/^{90}Y beta source to assess dosimetrics features. Particles obtained were characterized using IR, SEM/EDX, and TEM.

The results of TEM analysis suggested that particles sizes were ranging from 14 to 241 nm. The EDX elemental composition analysis of the material revealed that the oxygen (~43%) and silicon (~24%) elements were the main component confirming the presence of silica in the material.

Samples were irradiated at doses from 1 to 300 Gy. The intensity of the peak increased with dose. The dose response exhibited a nonlinear behaviour. The superlinearity index evaluation demonstrated that the dose response was superlinear.

The material used in this study shows promising properties for use for radiation dosimetry.

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Electron Nano-Analysis of MOF Glasses

Robert C. Carroll[a]*, Sean M. Collins*[a]

[a]School of Chemical and Process Engineering, University of Leeds, LS2 9JT, United Kingdom,
E-mail: R.C.Carroll@leeds.ac.uk, S.M.Collins@leeds.ac.uk

Keywords: metal-organic frameworks, electron diffraction, pair distribution function, amorphous materials

Metal–organic framework (MOF) materials have shown exciting performance characteristics across a tremendous range of applications, from chemical separations to catalysis [1-2]. Yet a long-standing challenge for commercialisation of MOFs, typically produced as crystalline powders, remains processability and integration in monolithic form. Recent progress in the fabrication of MOFs as monolithic glasses and glass composites offers a key route to the desired form factors for use in devices [3]. These MOF glasses, though, contain incredible structural variety and the mechanism of crystal-to-amorphous transition is not well defined.

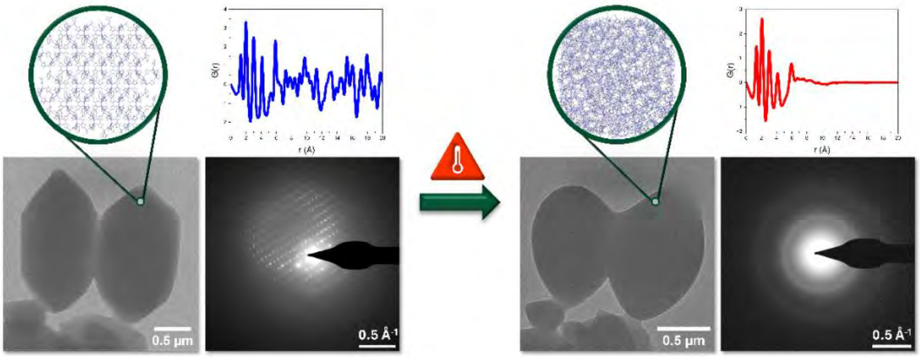

Figure 1: Schematic of *in situ* crystal-to-amorphous phase transition assessed by ePDF.

Our work seeks to understand the amorphous structure of melt-quenched glassy MOFs and the phase transitions they undergo, using nanobeam electron scattering methods in the scanning transmission electron microscope (STEM). The balance of spatial and momentum transfer resolution offered by nanobeam diffraction enables mapping of structural heterogeneity and complementary crystallographic analysis. Moreover, nanobeam electron scattering can be carried out under low-dose conditions, suitable for beam-sensitive MOF materials [4], and supports simultaneous amorphous structure analysis through electron pair distribution function analysis (STEM-ePDF).

Preliminary studies have focused on zeolitic imidazolate framework-62, a well-known glass-forming MOF, for optimisation of ePDF acquisition. This analysis aims to identify limits for real-space peak resolution and maximise detection of real-space pairwise correlations, whilst also studying dynamic structural transitions of glassy MOFs. Data acquired at multiple temperatures, *in situ* and *ex situ*, has indicated intermediate material heterogeneity and evaluation of surface melting mechanisms is being undertaken. Modelling of systems with electron scattering factors will enable quantitative assessment of ePDF profile fitting and multiple scattering contributions. Further developments seek to define spatially varying amorphous features and improve understanding of strain induced by glass formation.

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Topochemical postulates in action: comparative analysis of solid-state Diels-Alder reactions between similar charge transfer co-crystals

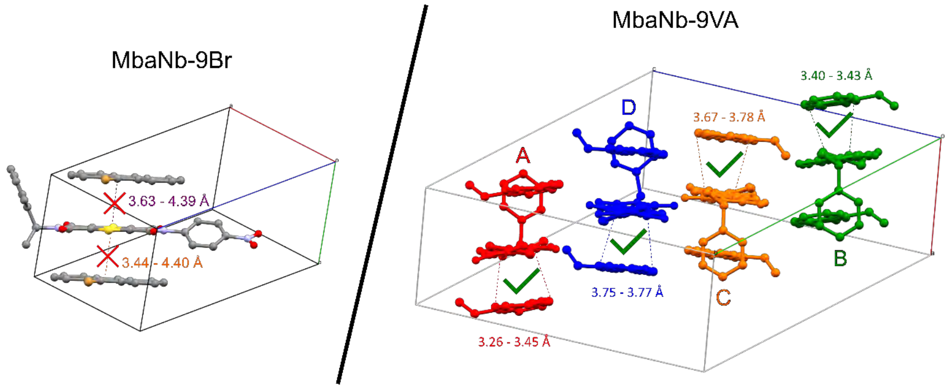
Tracy A. Lau[a], Demetrius C. Levendis[a] and Manuel A. Fernandes[a]

[a] Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, PO WITS 2050, South Africa. Email: tracy.lau@wits.ac.za

Keywords: crystal engineering, solid-state reactions, single crystal X-ray diffraction

Sustainable green chemistry is on the rise, as we see negative impacts on the climate, a depletion in the amount of non-renewables resources and excessive amounts of toxic waste products produced.[1] Solid-state reactions can be a way to alleviate the large use of solvents found in traditional synthesis, as well as efficiently produce regio- or stereospecific products.[2] Molecules can be engineered to arrange within a crystal lattice in such a way to undergo reactions initiated under light or heat by manipulating their intermolecular forces.[3] This can also be seen in the formation of co-crystals, where two different molecules are held together through non-covalent bonds, forming a crystal lattice of alternating molecules that can undergo chemical reactions.[4] Possible reactions within a crystal usually meet Schmidt's criterion, where the reacting molecules are aligned in parallel and within 4.2 Å of each other, undergoing minimal movement when reacting.[5] However, some crystals that meet these requirements still do not react or lose their crystal integrity over the course of conversion.

Two different charge transfer (CT) co-crystals were formed using (*N*-(*S*)-(-)-α-methylbenzylamino, *N*-paranitrophenyl)-1,4-dithiin (MbaNb) as the electron acceptor, with either 9-bromoanthracene (9Br) or 9-vinylanthracene (9VA) acting as the electron donor. Both co-crystals formed a 1:1 donor to acceptor CT stack, with the potential to undergo a Diels-Alder reaction. MbaNb-9Br formed in monoclinic $P2_1$ while MbaNb-9VA crystallized as triclinic *P*-1. However, only MbaNb-9VA underwent a Diels-Alder reaction while MbaNb-9Br remains stable at various temperatures. The differences and similarities between both CT co-crystals will be explored in detail.



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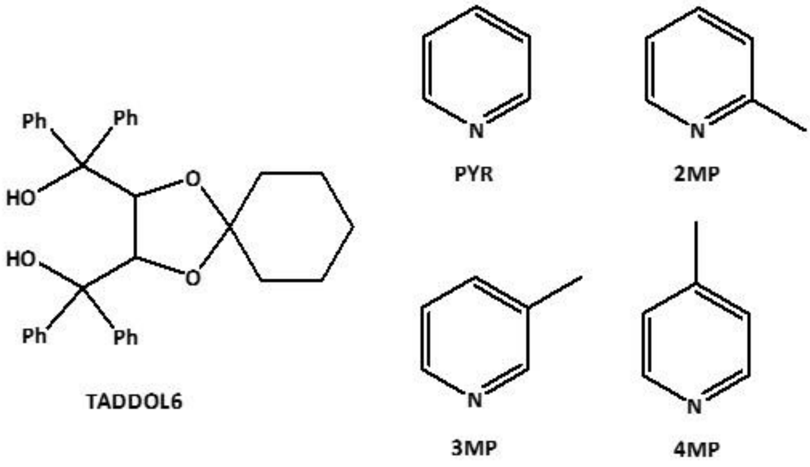
Extremely effective separations of pyridine/picoline mixtures through supramolecular chemistry employing TADDOL6 as the host compound

Daniella L. Recchia, Benita Barton and Eric C. Hosten

[a] Department of Chemistry, Nelson Mandela University, PO Box 77000, Port Elizabeth, 6031, South Africa.
E-mail: s220241104@mandela.ac.za

Keywords: selectivities, supramolecular chemistry, host–guest, green

The present investigation focussed on assessing the ability of (4*R*,5*R*)-bis(diphenylhydroxymethyl)-2-spiro-1′-cyclohexane-1,3-dioxolane (TADDOL6) to separate pyridine/methylpyridine (picoline) mixtures through supramolecular chemistry protocols. At the outset, TADDOL6 was revealed to possess the ability to form 1 : 1 host : guest inclusion compounds with each of pyridine (PYR) and 2-, 3- and 4-methylpyridine (2MP, 3MP and 4MP) in single solvent crystallization experiments. This host compound, furthermore, demonstrated enhanced selectivities in PYR/MP mixtures: preferred guests were PYR and 3MP (in the absence of PYR), followed by 4MP and then 2MP. Subsequent binary guest competition experiments showed that TADDOL6 may be employed in order to effectively separate very many of these mixtures in this way, and significant selectivity coefficients (*K*) were calculated in numerous instances. Single crystal X-ray diffraction (SCXRD) experiments showed that the only significant (host)π···π(guest) stacking interactions were those between TADDOL6 and the preferred PYR and 3MP guest molecules, while a consideration of Hirshfeld surfaces demonstrated that these preferred guests were involved in a tighter packing motif with TADDOL6 than those with 2MP and 4MP. Results from thermal analyses, more specifically when determining the guest release onset temperatures (T_{on}) and the enthalpies associated with these release processes, also agreed with the host selectivity order in the mixed guest competition experiments. The structure of TADDOL6 and the pydine/methylpyridines is illustrated in Scheme 1.



Scheme 1 Molecular structures of TADDOL6 and PYR and the three MP isomers.

Crystallographic characterization of solid oxide electrolytes.

David G. Billing[a]*, Caren Billing*[a] *,Sikhumbuzo M. Massina*[b]

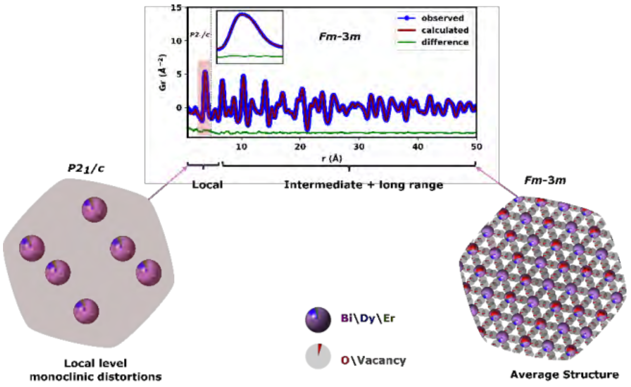
[a]School of Chemistry, University of the Witwatersrand, PO Wits, Johannesburg, 2050, South Africa,
E-mail: dave.billing@wits.ac.za.
[b]SSRL, SLAC National Accelerator Centre, Menlo Park, California, 94025, USA

Keywords: Bismuthate, Solid Oxide Electrolyte, XRD, PDF

Solid oxide electrolytes find application in SOFC's, SOEC's, oxygen sensors and similar devices. These and related functional materials are all structurally and compositionally complex and to unravel the crystallographic details underpinning a specific materials' key structure-properties-performance require the use of a number of more advanced powder diffraction and synchrotron measurements and data analysis methodologies.

Within this context our research has focused on gaining a fundamental understanding of the mechanisms governing the transport properties of these and closely related materials such as δ-Bi_2O_3 which has the highest reported oxides ionic conductivity for the $(BiO_{1.5})_{0.88}(DyO_{1.5})_{0.08}(WO_3)_{0.04}$ case [1], as well as the role of the various doped variants in these structure-property relationships. Typically, the cubic forms of these materials exhibit higher oxygen ionic conductivity due to the presence of vacant anionic sites, and exists only at elevated temperatures. In most cases doping results in only a meta-stable cubic phase that slowly transitions to a less conducting phase. From a collection of almost 400 distinct chemical compositions we have learnt that the nature, number and concentration of the dopents used, all affect the conductivity and stability of the desired phase in a complicated manner.

As part of our studies we performed variable temperature near simultaneous XRD and Total scattering measurements at NSLS-II, High resolution XRD at SSRL. This complements our lab-based VT-XRD, VT-EIS and VT-Raman measurements. Preliminary qualitative assessment of these results as well as some selected XAS measurements, readily suggests the difference and importance of local structural details as compared with the average crystal structures. For a more detailed crystallographic understanding we further analysed/modelled our measurements using sequential and symmetry constrained Rietveld methods, Real space modelling of the PDF's as well as Reverse Monte Carlo atomistic modelling. Here we would like to present the results of our studies on various Bismuthate materials



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Substantial Impact of Ligated Solvents on the Degree of Interpenetration Controlling CO_2 and Water Sorption Hysteresis in Isoreticular MOFs

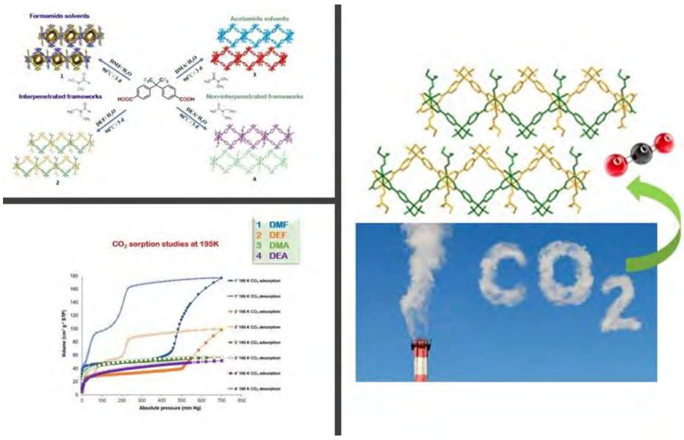
Nabanita Chatterjee[a] *and Clive L Oliver*[a]

[a] Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa, E-mail: n.chatterjee@uct.ac.za

Keywords: metal-organic frameworks (MOFs), polymers, interpenetration, carbon dioxide sorption studies, hysteresis, crystallography, diffraction

Metal-organic frameworks (MOFs) are considered a promising class of porous materials that consists of single metal ions or clusters which are linked by organic ligands into 1D, 2D, or 3D coordination polymers with potential voids with versatile applications in separation chemistry, catalysis, molecular sensing and gas storage.[1] Void volumes are often controlled by a physical phenomenon known as interpenetration, where at least two framework in a structure are entangled with each other in an inseparable way except breaking any covalent or coordination bonds.[2] In this study, the synthesis and sorption properties of two pairs of isoreticular Cu(II)-based 2D MOFs employing the bent ligand 4,4′-(hexafluoroisopropylidene)bis(benzoic acid) (H_2hfipbb) have been reported.[3] The first pair of MOFs, $[Cu(hfipbb)(DMF)]_n.0.5(DMF)_n$ (**1**) and $[Cu(hfipbb)(DEF)]_n$ (**2**), are formed when the formamide solvents *N*,*N*′-dimethylformamide (DMF) and *N*,*N*′-diethylformamide (DEF), respectively, are employed and are doubly interpenetrated. While the second pair of MOFs, $[Cu_3(hfipbb)_3(DMA)_3]_n.6(DMA)_n{\cdot}2(H_2O)_n$ (**3**) and $[Cu_3(hfipbb)_3(DEA)_3]_n.6(DEA)_n{\cdot}2(H_2O)_n$ (**4**), are formed when the acetamide solvents *N*,*N*′-dimethylacetamide (DMA) and *N*,*N*′-diethylacetamide (DEA) are employed and are non-interpenetrated.

Unexpectedly, the doubly interpenetrated structures exhibit superior carbon dioxide and hydrogen sorption properties compared to their non-interpenetrated counterparts, despite possessing much lower potential void volumes. Our findings further reveal that the identity of the solvent ligand in the as-synthesized MOF not only influences whether interpenetration occurs but also dictates the sorption sequence within an isoreticular pair. These results highlight the pivotal role of the solvent ligand in shaping the activated MOF’s structure and, consequently, its gas sorption behaviour.



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Application of BSA-conjugated AgInS/ZnS QDs for Electrochemical Sensing of Vascular Endothelial Growth Factor

N.A. Vitshima [a], *M.C. Matoetoe* [a], *N. Tsolekile*[a]*

[a]Department of Chemistry, Cape Peninsula University of Technology, Western Cape, South Africa, P.O. Box 652, Cape Town 2000, South Africa; E-mail: Vitshimaanathi@gmail.com

Keywords: AgInS/ZnS, BSA, bioconjugate, electrochemical biosensor and VEGF

AgInS and AgInS/ZnS quantum dots (QDs) are ternary semiconductor nanocrystals that have unique optical and electronic features, including large Stokes shifts, long fluorescence lifetimes, and minimal bio-toxicity. The bioconjugation or surface modification of QDs with biomolecules improves their biological targeting and biocompatibility. Bovine serum albumin is a biocompatible biomacromolecule with multiple binding sites for transition metal ions that has been identified as a highly effective substrate to stabilize fluorescent/catalytic metal nanoclusters. In this study, we report the synthesis of water-soluble glutathione-capped AgInS core QDs and AgInS/ZnS core/shell QDs via a reflux method. The QDs were conjugated with BSA to form BSA-AgInS/ZnS QDs, and the developed conjugates were investigated as a potential immunosensor for the electrochemical detection of vascular endothelial growth factor (VEGF). Using differential pulse voltammetry (DPV) as a detection method, the synthesized BSA-AgInS/ZnS QDs VEGF immunosensor exhibited a linear response range of 0.003 to 0.017 µg/ml with a limit of detection (LOD) of 1.5 × 10-3 µg/ml and a quantification limit (LOQ) of 5 × 10-3 µg/ml. Notably, the immunosensor maintained functional stability over five weeks, indicating potential for practical biosensing applications.

Calixarene-conjugated carbon dots for selective fluorometric detection of targeted pharmaceutical compounds in water

Clever Ng'andu and Sifiso A. Nsibande

[a] Department of Chemistry, Faculty of Natural and Agricultural Sciences, University of Pretoria, Lynnwood Road, Pretoria
Email: cleverngandu95@gmail.com

Keywords: antiretroviral drug, carbon dot, calixarene, fluorescence, sensor

Inadequate access to clean and safe drinking water remains a critical public health concern across the developing world, posing serious health risks, especially among children. This has been exacerbated by water pollution arising from various anthropogenic activities, including the expansion of chemical and pharmaceutical industries to meet the high demand for medical and personal care products [1]. Moreover, the high prevalence rate of infectious diseases like HIV/AIDs particularly in Southern Africa, has facilitated the introduction of emerging pharmaceutical products such as antiretroviral drugs (ARVDs) in water sources. These compounds enter the aquatic system primarily through human excretion, landfill leachate, discharge from healthcare facilities, and improper disposal of unused or expired medications. Prolonged exposure to these chemical species has been linked to adverse health complications in humans and inhibited growth in aquatic organisms [2,3]. This underscores the urgent need for robust and effective onsite monitoring systems for chemical pollutants in water sources. Herein, we report the development of a range of cost-effective and sustainable nanosensing tools, based on carbon dots (CDs) conjugated with calixarene (CA) supramolecular scaffolds. The CDs were prepared by bottom-up synthesis strategies, including hydrothermal and pyrolysis using citric acid and urea as carbon and nitrogen sources. Consequently, calixarenes and their derivatives were synthesized then covalently coupled with CDs by adopting a series of methods reported in literature. Characterisation of the resulting CD-CA nanoconjugates was then conducted using Fourier transform infrared (FTIR), nuclear energy resonance (NMR), transmission electron microscopy (TEM), energy dispersive spectroscopy (EDS), X-ray diffraction (XRD), UV-visible spectrometry and fluorescence spectrophotometry. The resulting CD–CA nanoconjugates integrate the intrinsic optical properties of CDs with the host–guest recognition capabilities of CAs to achieve selective interactions with pharmaceutical contaminants. Target analytes, including efavirenz, lamivudine, and naproxen were found to trigger distinct fluorescence responses of enhancement, quenching, and ratiometric shifts, respectively. Finally, the performance of these nanosensors in real-world samples was carefully evaluated.

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Microwave-assisted Synthesis of MOF-NiNPs@C for the Electrochemical Detection of Tramadol

Benneth C. Iwuoha[a,b], *Refiloe P. Modise*[a], *Siwaphiwe Peteni*[a], *Aderemi B. Haruna*[a] *and Kenneth I. Ozoemena*[a]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, PO Wits, Johannesburg 2050, South Africa.
[b]Nigerian Institute for Trypanosomiasis (and Onchocerciasis) Research (NITR), Federal Ministry of Science, Innovation and Technology, South - South Zonal Office, Federal Secretariat Complex, Okpanam Road, Asaba 320108, Delta State. Nigeria.
E-mail: 2937535@students.wits.ac.za

Keywords: MOF-derived nickel nanoparticles@carbon, tramadol, differential pulse voltammetry

Tramadol is a synthetic analogue of codeine, belonging to the family of opioid drugs. It is indicated for rapid onset analgesia in the peri-operative period, trauma or emergency unit, as well as in the intensive care and ward settings. If not properly regulated, it can lead to seizure, hypertension, psychiatric symptoms like hallucinations, panic attacks, which are life threatening.[1]

Unlike the traditional methods of drug detection, electrochemical sensors are attractive owing to their properties, such as low-cost, portability, and rapid responses coupled with the properties of metal organic framework derived nickel nanoparticles@carbon (MOF-NiNPs@C) which include large surface area, tunable porosity, high porosity, and the ability to incorporate various functional groups.

In this study, the use of glassy carbon electrode (GCE) modified with MOF-NiNPs@C was used in the electrochemical detection of tramadol.

The nickel-based MOF was synthesised via a microwave-assisted method, followed by calcination to yield the MOF-NiNPs@C. The nano-catalyst was characterized using XRD, SEM, HRTEM. The SEM of the nano-catalyst showed a spherical morphology. The XRD revealed that the nano-catalyst was metallic with face-centered cubic crystal structure.

Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were used for the electrochemical sensing, which reveals that the GCE modified with the nanoparticles (GCE-MOF-NiNPs@C) favours faster electron transport and electrocatalysis toward tramadol when compared with the bare GCE. The current evolutions from the scan rate studies show that the reaction is completely irreversible with a linear Randles-Sevcik plot showing a slope of 0.609, indicating mixed diffusion- and adsorption-controlled process. Further analysis showed Tafel Slope ($b = 0.198$ V) indicating good kinetics and charge transfer coefficient ($\alpha = 0.701$) indicating that the activation free energy curve for this reaction is asymmetrical. The GCE-MOF-NiNPs@C for tramadol detection, showed sensitivity of 18.881 uA/mM with limits of detection (LoD) and quantification (LoQ) of 31.0 µM and 10.0 µM, respectively. Furthermore, sodium dodecyl sulphate (SDS) was used to enhance the sensitivity of the sensor. The GCE-NiNPs@C+SDS showed an increased sensitivity of 99.431 µA/mM with LoD and LoQ of 3.40 µM and 11.0 µM, respectively. In the presence of interferants such as uric acid, acetaminophen, the tramadol was still detectable.

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Computation for a green future: exploring the catalytic conversion of methane.

Matthew G. Quesne[a]

[a] School of Chemistry, University of Leeds, Leeds, United Kingdom, E-mail: m.g.quesne@leeds.ac.uk

Keywords: Computational Chemistry, Green Chemistry, Sustainable Chemistry.

Methane emissions now account for ~30 percent of anthropogenic warming, therefore, centralised methane capture and conversion is an extremely promising technology for future green chemistry research. This talk will explore methane conversion by: (1) the photoactive covalant framework material CFT-1[1] and (2) Au supported on ZSM-5.[2]

Materials and Methods: CFT-1: Catalyst activity of CTF-1 is compared to: (1) Anatase TiO_2 and (2) g-C_3N_4. The photocatalytic reactions are carried out under irradiation by a 365 nm LED source. Au-ZSM-5: H-ZSM-5 with SiO_2/Al_2O_3 ratio of 25 is loaded with Au by deposition–precipitation. Methane oxidation is carried out in an autoclave reactor. It was determined that Fe-leaching from this reactor partially coated Au-particles but had no effect on catalysis. Computation calculations for both systems used Density Functional Theory (DFT) in combination with Perdew−Burke−Ernzerhof functional (PBE), as implemented in the Vienna Ab initio simulation (VASP) code.

Results and Discussion CFT-1: This study demonstrates that the intrinsic molecular heterojunction in the CTF-1 polymer is highly selective for solar-driven methane transformation towards ethanol. At a GHSV of 2000 mL h^{-1}, the photocatalytic methane-to-ethanol conversion at 65 °C represents a very high selectivity of ca. 80 % and a yield of 122.4 mol h^{-1}. The study rationalises a process for methane transformation to ethanol via ethane, without the over-accumulation of strong oxidants, seen in C_3N_4-based catalysts. Au-ZSM-5: This study showed that Au nanoparticles supported on ZSM-5 can oxidise CH4 to methanol and acetic acid with minimal formation of CO_2. In the batch experiments, a maximum oxygenate productivity was observed of 7.3 mol Au–1 h–1. This is much higher than that reported for the exemplar Cu-based catalysts tested under similar flow conditions.[3] In contrast to the Cu-zeolite catalysts, for which only C1 products are observed, C2 oxygenates are the major products observed with the Au-ZSM-5 catalyst, demonstrating that the Au catalyst operates by a different mechanism.

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Computational Study of Azobenzenes as Cholesterol Lowering Drugs.

Menezi Tshaka[1], Kabelo Mokgopa[1], Nomampondomise Molefe[1], Tendamudzimu Tshiwawa[1]

[1] Rhodes University, Chemistry Department, Makhanda, Eastern Cape, South Africa, E-mail: menezimentra@gmail.com.

Keywords: Cholesterol, Cardiovascular Diseases, Molecular Docking, Molecular Dynamics

Fatalities due to cardiovascular illnesses account for over 32% globally, positioning CVDs as one of the World's major causes of mortality. A common cause of in these diseases is the excess cholesterol in the body, which results in the build-up of plaque in and on the artery walls. The build-up is through a process called atherosclerosis. The accumulation of cholesterol deposits causes arterial stenosis, narrowing the vessel lumen and restricting the flow of oxygenated blood throughout the body[1]. The current treatment for these conditions (statins) targets inhibition at the early stages of cholesterol biosynthesis, depriving the body of other vital sterols from the pathway and causing several side effects in patients[2]. This study strategically targets the last stages of cholesterol biosynthesis with the objective of identifying azobenzene derivatives that demonstrate best binding affinity compared to native ligands of key biosynthetic enzymes. Specifically, the manuscript focuses on five critical proteins involved in cholesterol production, which include Squalene Monooxygenase (PDB ID: 6C6N), Lanosterol Synthase (1W6K and 1W6J), Sterol 14α-Demethylase (3K1O), and Cytochrome P450 51 (1H5Z). Through rigorous molecular docking analyses, several azobenzene-based compounds from the screened library exhibited stronger binding interactions than the native ligands across all five target proteins, suggesting their potential as potent inhibitors. Subsequent molecular dynamics (MD) simulations further validated the stability of these protein-ligand complexes, revealing that the ligands maintained consistent binding without undergoing significant conformational fluctuations over time. These findings collectively provide supporting evidence for the viability of azobenzene derivatives as promising cholesterol lowering drugs.

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Computer-Aided Catalyst Design: Organic Catalysts for CO_2 Conversion into Urea

Morad M. El-Hendawy

[a] Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg 2050, South Africa, E-mail: morad.el-hendawy@wits.ac.za.

Keywords: CO_2, Urea, DFT, Organic Catalyst, Reaction Mechanism

South Africa faces three pressing environmental and economic challenges: (1) rising atmospheric CO_2 levels, driving climate change; (2) NH_3 pollution, a significant environmental threat; and (3) increasing demand for urea-based fertilizers to support its vital agricultural sector, crucial for food security and economic stability. Conventional urea production relies on the Haber-Bosch process, an energy-intensive method that generates substantial CO_2 emissions. This study proposes a sustainable and innovative approach, employing green catalysts to convert atmospheric CO_2 and NH_3 into urea through environmentally friendly catalytic processes. By leveraging advances in computational chemistry, the research focuses on the design and optimization of efficient organic catalysts. The ideal catalysts are strongly nucleophilic, stable under reaction conditions, selective toward urea formation, and reusable. In this context, new N-Heterocyclic Carbene (NHC) catalysts were investigated computationally, revealing that they are excellent CO_2 activators, forming stable carbene–CO_2 adducts that react with amines to produce urea-like compounds. These findings provide a foundation for future experimental validation and the development of sustainable CO_2-to-urea conversion technologies.

Half-sandwich pyrazolyl-functionalized Ru(II)-NHC complexes: synthesis, characterization, antibacterial and DFT studies

Ngonidzashe Ruwizhi[a], *Sithabile Mokoena*[b], *Thishana Singh*[a], *Bernard Owaga*[a] *and Muhammad Bala*[a]

[a] School of Chemistry and Physics, University of Kwazulu Natal, Westville campus, Durban, South Africa. 222128440@stu.ukzn.ac.za. [b]School of Health Sciences, University of Kwazulu Natal, Westville campus, Durban, South Africa.

Keywords: N-heterocyclic carbene, S. aureus, antibacterial, DFT

Antimicrobial resistance has emerged as a global health threat, and recent estimates indicate a growing trend in antibiotic resistance, with thousands of deaths reported annually [1]. This has necessitated research into potentially more effective antimicrobial agents [2]. In this study, 10 novel pyrazolyl-functionalized Ru(II)-NHC complexes were synthesized, with varying substituents such as N-wingtips on the azolium moiety, simple imidazolium and benzimidazolium moieties and different carbon chain lengths on the pyrazole moiety. All the compounds were fully characterized by spectroscopic and analytical means. SC-XRD structures showed the complexes to correspond to the proposed structures of piano-stool style, with the azolium ligand being bidentate.

In vitro studies showed the Ru(II)-NHC complexes to have moderate antibacterial activity in the range of 88-403 µM, which was comparable to some complexes of the same nature reported in literature [3][4]. Computational DFT predictions complemented with the experimental findings. Both the HOMO and LUMO were found to be lying on the p-cymene, metal centre and chloride ligands. Molecular electrostatic potential maps showed the complexes to be more electron acceptors than donors, with the regions around the chloride ligand and metal centre having some electron donating ability. The benzimidazolium-based Ru(II)-NHC complexes with ethyl substituents on the pyrazolyl moiety exhibited the highest antibacterial activity. This might be due to the presence of long carbon chains which are known to enhance lipophilicity which ultimately improves antibacterial activity [5].

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Room Temperature Detection of *Aspergillus flavus* Volatile Organic Compounds under simulated conditions using GO and SnO_2 NRs

Viola O. Okechukwu[a], *OJ Okonkwo*[a], *Abidemi P. Kappo*[b], *Patrick B. Njobeh*[c], *and Messai A. Mamo*[d]

[a] Department of Environmental, Water and Earth Sciences, Tshwane University of Technology, Arcadia Campus, Private BagX680, Pretoria 0001, South Africa.
[b] Department of Biochemistry, Auckland Park Kingsway Campus, University of Johannesburg, South Africa.
[c] Department of Biotechnology and Food Technology, PO Box 17011, Doornfontein Campus, University of Johannesburg, South Africa.
[d] Department of Chemical Sciences, PO Box 2028, Doornfontein Campus, University of Johannesburg, South Africa.

Keywords: gas sensor; graphene oxide; SnO_2 NRs; organic compounds; hexanal; octanal; benzaldehyde

Volatile organic compounds (VOCs) are organic chemicals that are released from environmental pollutants or living organisms at high vapour pressure. This study investigated the application of a hybrid nanocomposite comprising tin oxide nanorods (SnO_2 NRs) and graphene oxide (GO) for the chemoresistive detection of selected volatile compounds (hexanal, benzaldehyde, octanal vapours) emitted by *Aspergillus flavus* under simulated conditions. These organic compounds were seleted based on their toxicological characteristics such as irritation to the skin, eyes, and respiratory tract, with octanal additionally capable of inducing allergic skin reactions. The synthesised hybride composite materials were characterised using various analytical techniques, including high-resolution transmission electron microscopy (HR-TEM), X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, X-ray diffraction (XRD), Brunauer-Emmett-Teller (BET) analysis, and Fourier transform infrared spectroscopy (FTIR). The results revealed that SnO_2 NRs alone exhibited limited sensing performance, while GO-based sensors responded to various analyte vapours. Incorporating SnO_2 NRs into GO matrix resulted in synergistic effects and improved sensor performance parameters including sensitivity, selectivity, response and recovery times were quantitatively determined from response curves. The SnO_2 NRs/GO nanocomposite demonstrated improved stability, sensitivity and good selectivity towards the targeted VOCs with acceptable response and recovery times. The sensor showed robust performance under relative humidity levels of up to 62%, achieving detection limits of 0.3 µg/kg for hexanal, 0.4 µg/kg for benzaldehyde, and 1.9 µg/kg for octanal. This study demonstrated the potential of SnO_2 NRs-GO composite-based sensor as a sensitive, selective and stable platform for VOC detection, with significant implications for both food safety and environmental monitoring applications.

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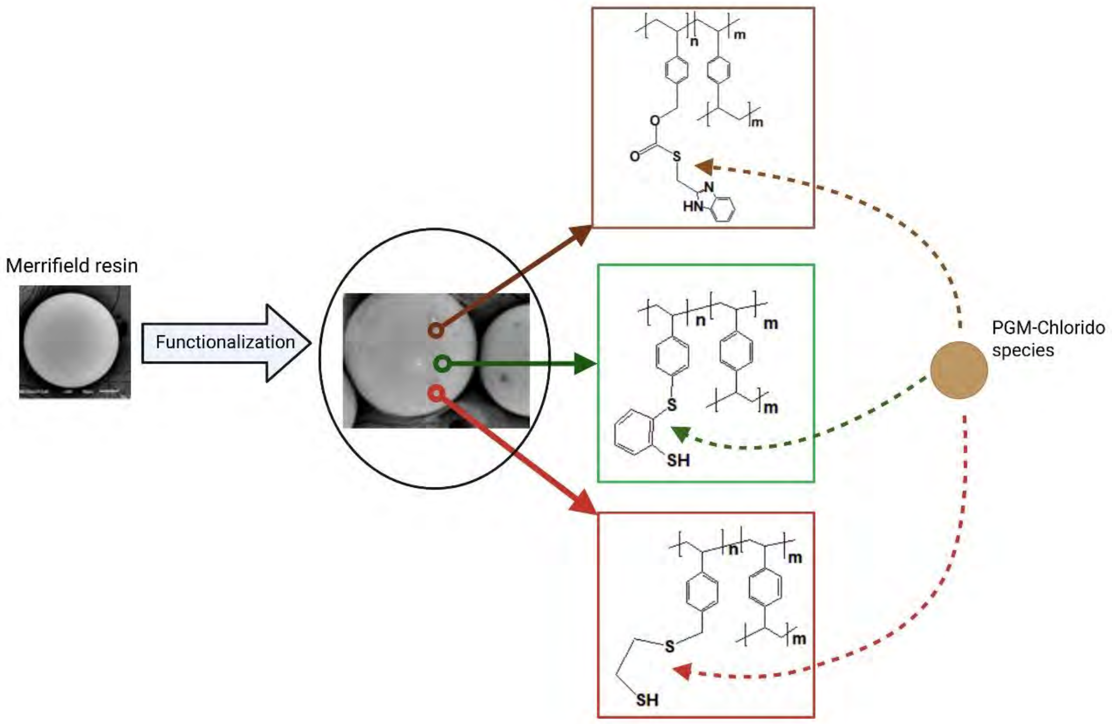
Selective Recovery of Palladium(II) Using Dithiol- and Benzimidazolylthio-Functionalized Merrifield Resins

Masivuye M. Mahleba, Jean-Luc Mukaba and Zenixole R. Tshentu [a]

[a] Department of Chemistry, Nelson Mandela University, P.O. Box 77000, Gqeberha 6031, South Africa

Keywords: palladium recovery, functionalized resin, Merrifield resin, benzimidazolylthio-, adsorption

Functionalized Merrifield resins were prepared using three ligands: 1,2-ethanedithiol (M-EDT), 1,2-benzenedithiol (M-BDT), and 2-benzimidazolylmethylthioacetic acid (M-BITAA), and applied in the adsorptive recovery of Pd(II) from acidic aqueous solutions. The resins were characterized using FTIR, UV-Vis, SEM, TGA and CHNS analysis, confirming successful functionalization. M-BITAA exhibited the highest Pd(II) adsorption capacity (0.247 mmol·g^{-1}), followed by M-EDT and M-BDT. Adsorption followed the Langmuir isotherm, and kinetic analysis showed good fit to pseudo-second order and Elovich models. Thermodynamic parameters indicated exothermic and enthalpy-driven adsorption, with the strongest spontaneity observed for M-BITAA. Selectivity studies revealed that M-BITAA favoured Pt(IV) over Pd(II), but exhibited high selectivity for Pd(II) over Ir(III), suggesting promise in multi-metal PGM separation from acidic media[1].



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Photoisomerization, Rotameric Conformational Behavior, Computational Insights, and Antiplasmodial Activity of Cinnamoyl–Chloroquine Hybrids

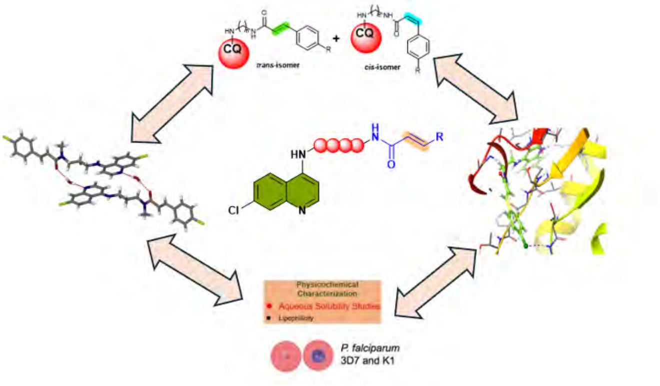
Mpelegeng V. Bvumbi[a], *Anza Nemudzivhadi*[a], *Simon Moleele*[a], *Mofeli Leoma*[b], *Dale Taylor*[c]

[a] Department of Chemistry, Faculty of Science, Engineering and Agriculture, University of Venda, Thohoyandou, 0950.
E-mail: Mpelegeng.Bvumbi@univen.ac.za.
[b]Department of Chemistry, Rhodes University, Makhanda, 6140, RSA.
[c]Holistic Drug Discovery and Development Centre (H3D), University of Cape Town, Rondebosch 7700, RSA.

Keywords: Cinnamoyl-chloroquine hybrids, Conformational analysis, Drug design, *Plasmodium falciparum*

Due to the emergence of *Plasmodium falciparum* strains resistant to both chloroquine and Artemisinin-based Combination Therapy (ACT) [1,2], significant efforts have been directed toward the discovery of novel compounds with potent antimalarial properties. Among the promising strategies is the design of molecular hybrids, particularly those in which two pharmacophoric moieties are covalently linked into a single entity, often resulting in improved efficacy compared to the parent drugs.

Cinnamoyl–chloroquine hybrids represent a promising chemotype in the search for new antimalarial agents, particularly against chloroquine-resistant *strains of Plasmodium falciparum*. In this study, a series of hybrids were synthesized and structurally modified to explore their conformational behavior, specifically the presence of rotamers, and their responsiveness to photoisomerization under UV irradiation. NMR spectroscopy and computational studies confirmed the existence of stable rotameric populations in solution, influenced by steric and electronic features around the amide bond. UV-induced cis/trans isomerization was monitored and correlated with changes in biological activity. Notably, certain irradiated forms demonstrated enhanced antiplasmodial efficacy, suggesting that light-induced conformational changes could be a novel strategy for modulating activity. These findings underscore the interplay between conformational dynamics and biological activity.



A schematic representation of the study.

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Solution-processed low-dimensional carbon materials via reductive dissolution

George Bepete[a]

[a] Department of Chemical and Materials Engineering, Department of Physics, and Centre for NanoScience Research (CeNSR), Concordia University, 7141 Sherbrooke Street West., Montreal, H4B 1R6, Canada, E-mail: george.bepete@concordia.ca.

Keywords: potassium, reductive intercalation, exfoliation, dissolution, graphene, graphene quantum dots

Alkali metal intercalation has emerged as a powerful strategy for transforming layered materials into solution-processable building blocks, enabling efficient exfoliation into high-quality nanosheets without harsh sonication or surfactant stabilization.[1] By introducing negative charge into layered materials such as graphite, intercalation converts otherwise rigid solids into polyelectrolyte salts that spontaneously dissolve in polar solvents, yielding dispersions of electron-rich nanosheets that can be directly integrated into functional devices. In this presentation, I will highlight three examples. First, potassium-intercalated graphite (KC_8) is exfoliated in tetrahydrofuran and transferred into water, producing surfactant-free dispersions of graphene suitable for fabricating homogeneous graphene films and graphene/MoS_2 heterostructure films.[2] These solution-processed films display strong interlayer coupling, enhanced optical absorption, sensitive dopamine detection, and capacitance values up to 38.3 F g^{-1} in non-aqueous electrolytes. Second, anthracite coal is transformed into a stage-I K-intercalated salt that dissolves spontaneously in polar aprotic solvents, yielding uniform sub-5 nm graphene quantum dots (GQDs) with narrow size distributions, strong excitation-dependent photoluminescence, and nonlinear thermo-optical properties.[3,4] Finally, applying similar reductive dissolution principles, we achieved the individualization of carbon nanothreads in polar media, producing stable dispersions that open new routes to process these one-dimensional sp^3 carbon nanomaterials for device fabrication.[5] These studies establish reductive intercalation as a versatile platform for producing scalable, high-quality low-dimensional carbon materials, opening new opportunities in solution-processed electronics, sensing, and energy storage.

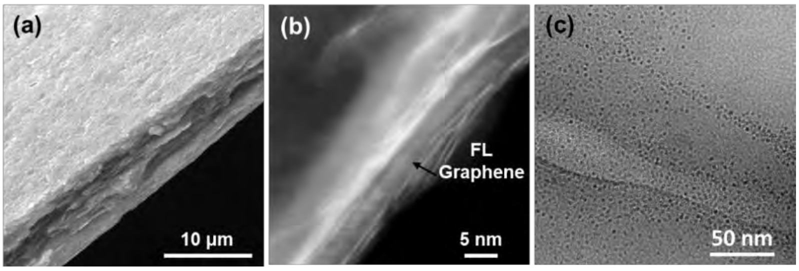

Figure 1. Cross sectional microscopy imaging of graphene/MoS_2 heterostructure films. (a) SEM Image. (b) HR-TEM image showing graphene sandwiched between MoS2 layers. (c) TEM image of coal derived graphene quantum dots.

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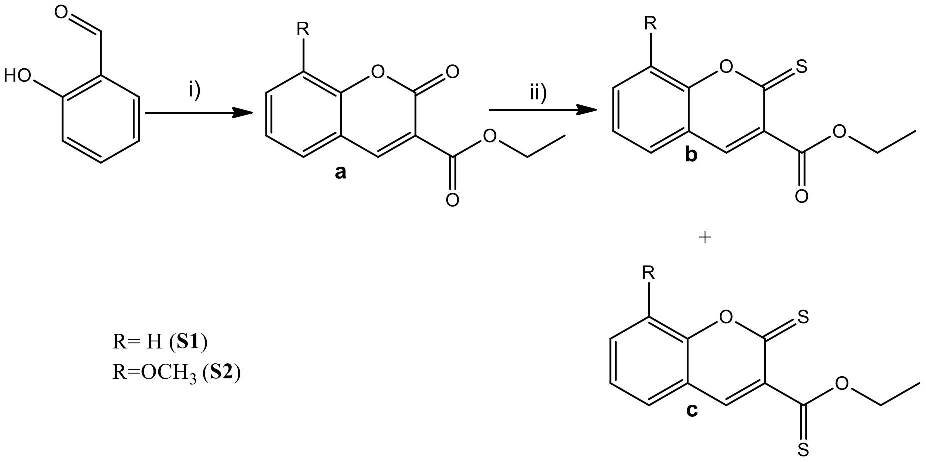
Design and synthesis of thiocarbonyl analogues of coumarin-based chemosensors with colourimetric properties: switching the selectivity from Fe^{2+}/Fe^{3+} to Hg(II) and Cu(II) ions

Lisa Myburgh, Stiaan Schoeman and Neliswa Mama

[a] Department of Chemistry, Nelson Mandela University, Gqeberha, Summerstrand, 6001, South Africa, E-mail: s219004889@mandela.ac.za

Keywords: Lawessons reagent, chemosensor, colourimetric, selectivities, mercury, copper, thionating

Lawesson's reagent is known as a thionating reagent, which is capable of converting a carbonyl or hydroxy functional group into its thio-analogue by replacing either the carbonyl oxygen or the oxygen from the hydroxy group with a sulphur atom. Compounds **S1a** and **S2a** were used to successfully synthesise and form their mono and disubstituted thio-analogues. It was noted that the carbonyl attached directly to the coumarin backbone was substituted first to form **S1b** and **S2b**. This was followed by the thionation of the carbonyl oxygen from the ester moieties attached to positions three of the coumarin backbone, subsequently forming compounds **S1c** and **S2c**. The thio-analogues were separated by means of preparative TLC using a dichloromethane: petroleum ether solvent mixture as the mobile phase (60:40). NMR, FTIR and elemental analysis were used to confirm the successful preparation of the sulphur-derived compounds. Compounds **S1a** and **S2a** were tested alongside their thio-analogues as potential chemosensors for metal ion detection in an acetonitrile solvent system. The unsubstituted coumarin-based compounds showed a unique selectivity towards both Fe^{2+} and Fe^{3+} metal cations, with an increase in the absorption of these chemosensors noted in their presence. In contrast, the mono and disubstituted thio-analogues showed great selectivity towards Hg^{2+} and Cu^{2+} ions. These compounds also exhibited colourimetric properties, with a change in colour from yellow to clear noted for both the mono- and disubstituted thiocarbonyl derivatives of **S1a** and **S2a** in the presence of Hg(II) and Cu(II) ions. [1, 2]



Scheme 1: General synthetic pathway used to synthesize compounds **S1a**, **S2a**,**S1b**, **S2b**, **S1c** and **S2c**. i) Diethyl malonate, piperidine, ethanol, glacial acetic acid, 2h reflux. ii) Lawesson's reagent, dry toluene, 8h reflux, N_2

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Untangling Complexity in Cola Beverages: A Non-Targeted GC-TOFMS Approach to Volatile Profiling and Unexpected Contaminant Detection

Christina Kannigadu[a], *Alexander Whaley*[a]

[a]LECO Africa, Gauteng, 1619, South Africa, E-mail: Christina@lecoafrica.co.za

Keywords: GC-TOFMS, Non-Targeted Analysis, Mass Spectrometry, HS-SPME, ChromaTOF Sync, Cola, PCA, Flavor Chemistry, Deconvolution

Non-targeted chemical profiling has become an increasingly valuable strategy in food and beverage analysis, particularly when characterizing complex matrices or uncovering previously unmonitored components. In this study, we employed Headspace Solid-Phase Microextraction (HS-SPME) coupled with Gas Chromatography–Time-of-Flight Mass Spectrometry (GC-TOFMS) to evaluate the volatile profiles of 13 commercially available Cola beverages. The data were processed using ChromaTOF® Sync, a multi-sample alignment and deconvolution tool that streamlines the detection of both common and unique features across large datasets.

This approach enabled the identification of over 150 compounds, including key flavorants and potential degradation products—revealing differences in formulation and possible indicators of product quality. The high-speed, full-spectrum acquisition capabilities of TOFMS also allowed for post-acquisition analysis of the data, leading to the unexpected detection of compounds associated with potential packaging-derived contamination, none of which were originally targeted. These findings highlight the broader analytical utility of the platform for quality assurance, authenticity verification, and trace-level impurity monitoring.

Principal Component Analysis (PCA) and trend mapping via ChromaTOF Sync further highlighted chemical similarities and distinctions between products—offering insight into brand differentiation strategies and formulation overlap. This workflow, while demonstrated here using Cola beverages, is broadly applicable to other challenging matrices across food, fragrance, pharmaceutical, and environmental domains.

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Determination of heavy and polycyclic aromatic hydrocarbons in soil samples witbank, south Africa

Malesole N Bucibo[a], *Zoleka Nqaba*[b], *Samson Akpotu*[b] *Fanyana Mtunzi*[a]

[a]Department of Natural Sciences, Vaal University of Technology, Gauteng South Africa;
"mail to: malesole@vut.ac.za"

Keywords: Characterisation**,** Mpumalanga, PAHs, sediments, heavy metals, and soil

Electricity-generating power stations are known to release PAHs and heavy metals into the soil and surrounding environment due to the incomplete combustion of coal. Our study was based in Witbank, South Africa, and the aim was to assess the influence of the power stations on the concentrations of the PAHs and heavy metals in the soils near them. This is because

soil contamination from polycyclic aromatic hydrocarbons (PAHs) and heavy metals released during the incomplete combustion of coal for electricity generation poses risks to humans and the environment. PAHs are known to have an ability to accumulate in the soil, contaminate the ecosystems, and ultimately enter the food chain, posing threats to plant and human health. On the other hand, heavy metals can affect the soil quality, reduce crop production, and pose risks to human health through the food chain and groundwater contamination.

Soil samples were collected at 0-15 cm depth around the mining area, industrial, residential, and agricultural areas. The pH of the soil and sediment samples was determined. The samples were analysed using the ultrasonic-assisted extraction (UAE) technique coupled with acidic silica gel clean-up before quantification with gas chromatography-mass spectrometry (GC-MS). Heavy metals were determined using acid digestion followed by using inductively coupled plasma (ICP-OES).

The pH of the soil indicated acidic to basic samples. XRD disclosed the presence of quartz, which FTIR also confirmed. The FTIR analyses further revealed the presence of hematite Fe_2O_3, kaolinite, quartz SiO_2 and the presence of carbon content was disclosed by a peak around 1621-1641 cm^{-1} which signifies the presence of C=C in aromatic compounds caused by the presence of aromatic carbon content.

PAHs identified include naphthalene, acenaphthene, fluorene, anthracene, fluoranthene, pyrene, and Benz[a]anthracene.

The PAHs concentration ranged between 140 and 2230 µ/kg. Selected heavy metals, namely Cobalt (Co), Chromium (Cr), Copper (Cu) Iron (Fe), Manganese (Mn), Lead (Pb), and Zinc (Zn) from the soil. The concentration of the heavy metals ranged between 25.6 -358 mg/kg.

Non-targeted profiling of volatile compounds for the authentication of honey origin

Samukelisiwe Nhlapho[a], *Sithandile Ngxangxa*[b], *and Abayneh Ambushe*[a]

[a]Department of Chemical Sciences, University of Johannesburg, PO Box 524, Auckland Park 2006, Johannesburg, South Africa; E-mail: samkenhlapho@gmail.com

Keywords: Adulteration, Authentication, Botanical origin, Geographical origin, GC-MS, Honey

Honey is susceptible to various forms of adulteration, including the mislabelling of its botanical and geographical origin [1]. Honey authenticity is a highly evolving field, with an increasing interest in the botanical and geographical origin issue [2]. As concerns around food fraud and traceability grow, the authentication of honey based on its origin has become increasingly important for ensuring quality and consumer trust. This study aims to develop and optimize a non-targeted GC-MS-based approach for the profiling of volatile compounds in honey, to establish chemical fingerprints that enable reliable authentication of its botanical and geographical origin. Evaluation of multiple sample preparation methods, such as liquid-liquid extraction (LLE) and solid-phase extraction (SPE), was performed for non-targeted analyses of a wide range of honey aroma compounds using Gas Chromatography–Mass Spectrometry (GC-MS). Sample preparation evaluation was performed through the evaluation of different organic solvent ratios with honey for the attainment of high extraction peak capacity using GC-MS. A combination of various solvents with varying polarities was assessed in order to achieve the optimum extraction conditions. The evaluation of various solvent combinations resulted in the identification of more than 50 aroma compounds, tentatively identified by means of mass spectra library search and retention index calculation. Interestingly, some aroma active compounds such as eucalyptol, encecanol, hydroxymethylfurfural, furfural derivatives, *cis-dihydro*-rose oxide, and paniculol were tentatively identified in honey using GC-MS. Several of these compounds are known for their floral properties of honey, thus contributing significantly to the basis for identifying the origin and differentiation of honey samples, which could lead to the sensory differentiation of honey. A detailed comparison of multiple sample preparation methodologies was performed in order to highlight the selectivities between the optimized sample preparation methods. The solvents that yielded better selectivity were methanol and water (1:1) for dilution and dichloromethane (DCM) for extraction. The above highlighted findings contribute to the development of a reliable, non-targeted approach based on the GC-MS method for the detailed chemical fingerprinting and authentication of honey.

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Development and application of “selective capture” derivatizing protocol for alcohols

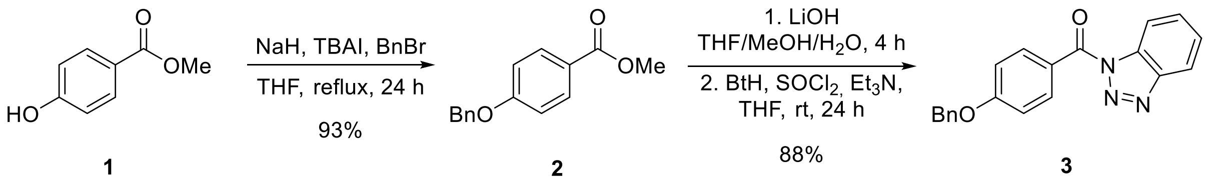
Mathew Khumalo[a], *Comfort Nkambule*[a]

[a]Department of Chemistry, Tshwane University of Technology, Private Bag X680 Pretoria, 0001, South Africa. E-mail: khumalomathew2@gmail.com

Keywords: 1,2,4-triols, *N*-acyl benzotriazole and regioselective derivatization

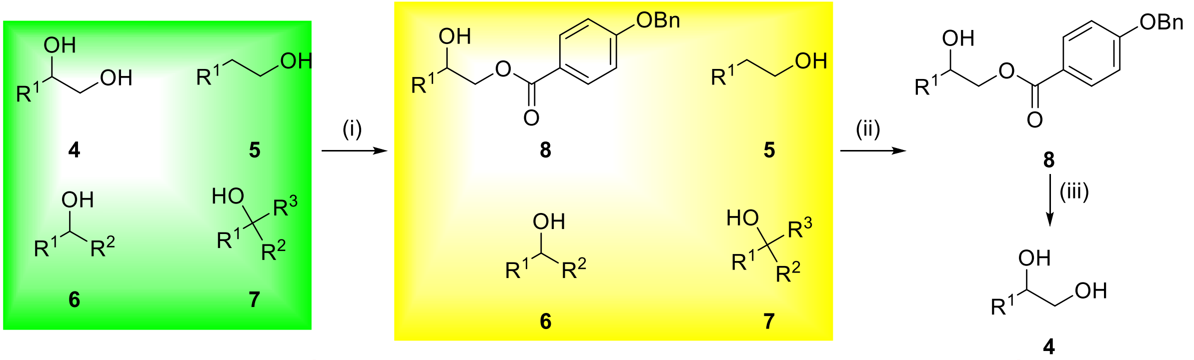
Synthetic organic chemists are interested in synthesizing naturally occurring compounds to supplement meagre sources from plants/animals or to modify them to produce novel molecules. [1] Compounds with 1,2,4-triol moieties are among desired targets due to their bioactivity against cancer, bacteria, fungi, and insects; these compounds can be synthesized or extracted from avocado seeds and leaves, but the extraction, isolation, and purification may be tedious and inefficient. [2] Thus, a smart derivatizing “tag, capture and release” protocol can expedite the isolation process, and be more environmentally friendly by reducing the numbers of purification steps.

The synthesis of crystalline and moisture-tolerant acylating agent **3** is shown in Scheme 1; this was accomplished in excellent yield (82%) from a commercially available starting material.



Scheme 1: Synthesis of an aromatic benzotriazole acylating group

The tagging agent **3** was successfully applied to the phishing of 1,2-diols (**4**) from a mixed matrix with primary (**5**), secondary (**6**), and tertiary (**7**) alcohols (Scheme 2).



(i) Selective derivatization (**tagging**); (ii) Preferential isolation (**capture**); (iii) Recovery deprotection (**release**)

Scheme 2 Application of the “tag, capture and release” derivatization protocol

The very crystalline nature of the tagging agent **3** greatly facilitates the isolation of the derivatized 1,2-diols, which are selectively acylated because of the tin acetal mediated regioselective reactivity of polyols.

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Development of multifunctional polymeric materials for controlled release in food and pharmaceutical applications

Wing-Fu Lai

[a] School of Food Science and Nutrition, University of Leeds, Leeds LS2 9JT, United Kingdom, E-mail: rori0610@graduate.hku.hk.

Keywords: polymers; controlled release; carriers; delivery; microencapsulation

Polymeric materials are an important class of materials that have attracted extensive research interest over the last several decades, owing to their high tunability in properties and the increasing sophistication of chemical and engineering techniques for polymer manipulation. In this presentation, I will introduce a self-indicating gel fabricated from a cellulose-based derivative for the controlled release of bioactive agents [1,2]. Increasing the polymer concentration was found to reduce swelling and erosion rates, thereby improving drug encapsulation efficiency and sustaining release. This also enhanced the gel's intrinsic luminescence and self-indicating capacity. Notably, the gel exhibited excitation wavelength-dependent emission, enabling flexible selection of excitation sources based on practical needs. In the *in vivo* context, the gel reduced the systemic toxicity of a chemotherapeutic agent and acted as a depot system that enhanced antitumor efficacy in both chemotherapy and immunotherapy settings [2–4], while also allowing real-time tracking of the gelation process and the location of the gel formed inside a living body [2]. Leveraging its controlled release, film-forming ability, and optical signaling, the polymer was further applied to food packaging. The resulting film demonstrated strong UV absorption in both UVA and UVB regions, protecting the packaged food from UV degradation while visually indicating film properties and food status. In addition to the cellulose-based system, I will also present how engineering techniques—particularly microfluidic electrospray—can be used to manipulate gel microstructures, enabling the effective co-delivery of drugs that may otherwise interact unfavorably upon direct contact. Together, these examples illustrate how integrated chemical and engineering approaches can potentially advance multifunctional polymer systems for smart, application-driven innovations.

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Abstract Title - Critical Differences in Analytical Techniques for the Analysis of Mercury in Waste for Landfill Disposal Assessment

Mahmood Patel[a]

[a]EnviroServ Waste Management, a Suez Company, Meadowdale, Germiston, Gauteng, 1614, South Africa,
E-mail: mahmoodp@enviroserv.co.za

Keywords: mercury, matrix effects, interferences, ICP-OES; ICP-MS, bias, reproducibility, volatility

The United States Environmental Protection Agency (US EPA) classifies mercury as a persistent, bio-accumulative toxin, indicating that its toxicity does not diminish through decomposition or chemical reaction, and that it is absorbed faster than it can be excreted.

The global focus on mercury management is reflected in the Minamata Convention on Mercury, an international treaty of which South Africa is a signatory, designed to protect human health and the environment from anthropogenic emissions and releases of mercury and mercury compounds. The year 2020 is a milestone for the Convention as this is when signatory parties are required to cease the manufacture, import and export of many mercury-containing products listed in the Convention.

Based on the above, efforts to minimize the release of mercury, and to track its migration when released, have demanded more sensitive analytical techniques for its measurement. As these techniques have become available, regulatory agencies around the world have written new analytical methods specifying their use.

Some of the preferred analytical techniques for measuring mercury include cold vapor atomic absorption spectroscopy (CVAAS), cold vapor atomic absorption fluorescence spectroscopy (CVAAF), and direct analysis by thermal decomposition. Most analytical laboratories in South Africa use either inductively coupled plasma optical emission spectroscopy (ICP-OES) or inductively coupled plasma mass spectrometry (ICP-MS) for measuring mercury.

Although some laboratories prefer to utilize inductively coupled plasma mass spectrometry (ICP-MS) for the determination of mercury, it does involve special sample handling including the addition of small amounts of gold to the sample to expedite baseline recovery. Moreover, the cost of such equipment can be as much as 3 to 5 times higher than dedicated CVAAS or CVAAF systems. Although inductively coupled plasma optical emission spectrometry (ICP-OES) based instruments can be used to measure mercury, trace level analysis is problematic due to poor sensitivity.

Experience has shown that the choice of analytical technique for accurate analysis is key to correct assessment for landfill disposal. The National Norms and Standards for the Assessment of Waste for Landfill Disposal (GN R. 365) section 3 clause (4)(2) prescribes that the standard assessment method for measuring total concentration of elements and chemical substances in waste must be determined using techniques and analysis methods that will provide reliable, accurate and repeatable results.

This paper will try to demonstrate how the differences in analytical techniques for the analysis of waste containing mercury can influence the landfill disposal assessment.

Development of the Multi-Purpose Reactor and the associated Beamline Facilities at the South African Nuclear Energy Corporation

Pradish Rampersadh

[a] Research and Innovation, South African Nuclear Energy Corporation, Elias Motsoaledi street, Pelindaba Madibeng, 0204, South Africa, E-mail: pradihs.rampersadh@necsa.co.za

Keywords: nuclear, research reactor, beamline science

The South African Nuclear Energy Corporation (NECSA) is the organ of state, mandated to undertake and promote research and development in the field of nuclear energy and radiation sciences and technology and to make these generally available. Necsa is also mandated to cooperate with any person or institution in matters falling within these functions. The corporation, have in the last few years redefined its strategic approach and will now be focusing on the following high impact areas:

- Re-establishing the front-end fuel supply for research and power reactors
- Focus on power generation with Small Modular Reactor technology
- Solidify neutron source generation (Safari 1 and the development of the Multipurpose Purpose Reactor
- Increase the footprint for radioisotope production
- Stabilize and develop the fluorochemical business
- Capacitation and strengthening skills development

The discussion will cover the above listed developments at Necsa and enlighten the chemistry community of possible opportunities in this space. There will be focus on the Development of the Multi-Purpose Reactor and the associated Beamline Facilities.

(NB: this is an information and not a scientific/technical presentation. There are substantial opportunities for the academic community to get involved in teaching and development)

The Role of Analytical Chemistry in a Decarbonising Petrochemical Industry

Boitumelo Makume[a], *Werner Welthagen*[a]

[a]Sasol Research and Technology, Klasie Havenga Road, Sasolburg, 1947, South Africa, E-mail: boitumelo.makume1@sasol.com.

Keywords: analysis, decarbonisation, feedstock, process, products

Analytical Chemistry plays a pivotal role in enabling Sasol's integrated value chain - from feedstock analysis, process analysis, emissions monitoring to final product specifications.

Many of the analytical methods used routinely are based on standard, internationally accredited methodologies. However, new and innovative analytical approaches are often required to address Sasol's unique process challenges. In addition, Sasol's current strategic ambitions to decarbonise operations, reduce greenhouse gas emissions and produce environmentally sustainable products introduces new and exciting challenges for the analytical chemist. This presentation will highlight a few of these examples.

Nanosilane-Modified Bitumen-Stabilized Base Materials: Mechanisms and Moisture Durability

Nikisha Sewpersad

[a] Tosas Wadeville, Germiston 1449 Gauteng, South Africa. E-mail: Nikisha.s@tosas.co.za

Keywords: nanosilane, bitumen-stabilized material, organosilicon, siloxane network, hydrophobicity, base construction, moisture resistance, adhesion

Nanosilanes—organosilicon compounds containing Si–O–Si and Si–C linkages—have demonstrated strong potential to improve the performance of bitumen-stabilized materials (BSMs) through surface modification and enhanced hydrophobicity. Their bifunctional molecular structure, consisting of hydrolyzable alkoxy groups (–OR) and organofunctional groups (e.g., amino, epoxy, vinyl), allows them to interact with both hydrophilic aggregate surfaces and hydrophobic bitumen.

Upon hydrolysis, the alkoxy groups form silanol (Si–OH), which condenses with hydroxyl sites on aggregates and fines to form a durable siloxane (Si–O–Si) network. This creates a hydrophobic mineral surface, significantly reducing moisture ingress and improving long-term durability [1]. At the same time, the organofunctional end of the molecule interacts with bitumen's polar constituents via hydrogen bonding and Van der Waals forces, enhancing interfacial adhesion and cohesion within the matrix. In road base applications, nanosilanes act as a molecular bridge, bonding aggregate to bitumen while forming a continuous water-repellent film that limits capillary suction and water infiltration.

The resulting siloxane–bitumen composite network increases strength retention and extends the service life of BSM layers. Nanosilane incorporation is especially beneficial in climates with variable moisture exposure or where aggregate quality is marginal. Nanosilane-treated BSMs can be considered cost-effective and a chemically effective alternative to conventional stabilizers for enhancing road base performance in challenging environments.

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Key Aspects of Pressurised Water Reactor (PWR) Chemistry for Safe and Reliable Operation

Nestor van Eeden

[a] Eskom, Koeberg Operating Unit, R27, off West Coast Road, Melkbosstrand, Western Cape, 7441, South Africa

Keywords: PWR, nuclear, reactions, water chemistry control, power plant

Chemistry control in PWRs is fundamental to safe, reliable, and efficient nuclear plant operation. This presentation outlines the key chemical parameters that govern primary and secondary circuit performance. In the primary system, emphasis is placed on pH_T control, lithium concentration, dissolved hydrogen, zinc addition, and boron management across the fuel cycle. For the secondary system, all-volatile treatment using advanced amine and ammonium chemistry is the focus, with specific attention to feedwater and steam generator pH control, oxygen and hydrazine management, and strategies to limit flow-accelerated corrosion. The impact of the primary and secondary chemistry regimes on materials performance, fuel integrity, and radiation field control will be highlighted, along with links to stress corrosion cracking, corrosion product transport, and steam generator tube integrity. By focusing on chemical agent parameter ranges, impurity control, and their operational significance, the presentation provides a high-level overview of the practices and challenges that underpin safe and reliable nuclear plant chemistry operation. In doing so, nuclear reactor chemistry not only underpins safe and reliable operation but also provides a ‘window for change’, driving innovation, strengthening sustainability, and contributing to global carbon reduction goals.

Rietveld refinement automation for process feedstock quality control (AUTO-INP) and other odd projects

Adam Shnier[ab], *Anzel Falch*[b], *David Billing*[b], *Caren Billing*[b] *and Daniel Wamwangi*[b]

[a] Xtal Insights, Johannesburg, South Africa, E-mail: adam@xtal-insights.ac.za. [b]Molecular Sciences Institute, School of Chemistry, University of Witwatersrand, Johannesburg 2050, South Africa.

Keywords: automation, diffraction, Rietveld, open-hardware

Large XRD data-sets are time consuming to work through for phase identification and Rietveld refinement. In the case of industrial feedstocks with continued monitoring, this can be a significant ongoing time-sink, limiting room for other more interesting work. To address such data-sets with identical phase composition can often be scripted with few challenges.

The reliability of simple scripting begins to fail in more variable and complex data-sets for which the presentation discusses. The methodology in developing a robust algorithm is discussed, including:

- Automated candidate phase identification from a user maintained database of probable structures,
- Identification of major and minor phases based on a user defined thresholds,
- Automated removal of false assignments at multiple stages,
- User assessment of output

This approach is built by interfacing with *launch mode* in Bruker's TOPAS software which provides a reliable and well validated basis [1].

In addition to the main topic a brief example of simple hardware solutions to technical problems faced in academia will be included.

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[1] Coelho, A.A. *J. Appl. Cryst*., 2018, **51**, 210-218. TOPAS and TOPAS-Academic: an optimization program integrating computer algebra and crystallographic objects written in C++.

Production of Sustainable Aviation Fuel from Fischer-Tropsch Wax - Understanding the interplay between product properties and product yield

Ryan Walmsley[a], *Maropeng Ngobeni*[a], *Delanie Lamprecht*[a], *Andile Mzinyati*[a]

[a]Sasol Research & Technology, Klasie Havenga Road, Sasolburg, 1947, South Africa, E-mail: ryan.walmsley2@sasol.com.

Keywords: SAF, Fischer-Tropsch, hydrocracking, power-to-liquids.

The Sasol-Topsoe G2L^{TM} process integrates high-efficiency syngas production, Fischer-Tropsch (FT) synthesis, and product upgrading to afford eFuels such as sustainable aviation fuel (SAF). Sasol's cobalt catalyst, characterised by high α_2 values, enables high yields of the long-chain hydrocarbons which in turn enables the production of superior SAF yields.

But how does the production of heavy wax afford high yields of a comparatively low boiling point jet fuel? This presentation will examine the upgrading of FT wax through hydroprocessing, focusing on the trade-offs in meeting jet specifications. Properties such as freezing point, final boiling point, and flash point govern the fraction of on-spec product. Achieving ultra-low freezing points (<-47 °C) requires significant hydroprocessing, but too severe and the resultant cracking to lighter products (naphtha, LPG) can lower jet yield. Insufficient branching, on the other hand, results in high freezing points limiting the carbon number range that can be incorporated into the final product.

Pilot plant testing has been conducted to quantify these relationships under representative conditions. The results illustrate how catalyst functionality, reaction severity, and distillation influence the achievable yield. Data from these trials will be presented to demonstrate the sensitivity of SAF yield to process variables. Beyond SAF, the unique molecular composition of Fischer-Tropsch wax also offers the potential to access additional high-value products, providing flexibility to align production with evolving market demands.

Beam line facilities at Necsa and their progression into the new multi-purpose reactor for material's analysis

Andrew Venter[a]

[a]Research and Innovation Division, Necsa SOC Ltd., Pelindaba, South Africa, E-mail: Andrew.Venter@necsa.co.za.

Keywords: Diffraction, Imaging, microstructures, in-situ investigations

The SAFARI-1 Research Reactor is a flagship nuclear facility with exemplary operational, maintenance and management records since its commissioning in 1965. SAFARI-1 facilities, complemented by X-ray based instruments, enables advanced materials characterization capabilities as probes of matter. Key techniques include powder diffraction for phase and structural analysis, micro-diffraction for strain scanning and preferred orientation assessments, as well as micro-focus X-ray imaging for high-resolution internal structure visualisation. These enable spatially-resolved characterisation of phenomena in materials and components, such as: Applied thermo-mechanical treatments for enhancing performance and application lifetimes; Component manufacturing technologies including additive manufacturing; Materials forming into billets used amongst others for the manufacture of aerospace components; Weldments in components; Energy storage systems including batteries and fuel cells.

Two world-class neutron diffraction facilities are applied to the applications neutron powder diffraction, PITSI instrument [1], and residual stress (micro diffraction), MPISI instrument [2]. These are equipped with an extensive suite of sample environments covering the range 1.5 K < T < 1800 K to facilitate in-situ studies of materials phenomena at resolution adequate for many structure refinement studies. In addition the modernisation of the neutron imaging capability is being finalised. These are all complemented with X-ray equivalent instruments.

All beam line instruments are generally accessible to the research community within the proposal-based User Access Program to beneficiate collaborative opportunities with subject matter experts from diverse scientific and engineering disciplines. An overview of the facilities, as well as recent collaborative projects, illustrating this, will be given.

This suite of neutron-based techniques will be substantially expanded with Necsa's future Neutron Beam Line Centre at the next generation Multi-purpose Reactor. This inevitably presents higher performance and technological advanced features to resolve even deeper insights of complex material systems and components. From the onset it will be equipped with thermal and cold beams extracted to experimental positions in the reactor beam hall, as well as an extended neutron guide hall areas. Neutron scattering features prominently to bring a suite of a world-class large-scale research infrastructure instruments to the fold. These are being determined in consultation with the User community, as well as with international expert inputs. Academia is seen as primary driver of this activity through their inherent alignment with the research and infrastructure mandates of relevant government departments. These new instruments substantially enhance the suite of investigative techniques available for scientific and technological research and development, in education and training programmes.

Various engagements are taking place to develop the neutron scattering community in SA.

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Silica-Anchored Acylthiourea and Amine Adsorbents for the Selective Recovery of Platinum and Palladium from Aqueous Media

Malehlogonolo R.R. Mphahlele[a], *Alseno K. Mosai*[b], *Hlanganani Tutu*[a], *Izak A. Kotzé*[a]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag X3, WITS, Johannesburg, 2050, South Africa. Email: Izak.Kotze@wits.ac.za. [b]Department of Chemistry, Faculty of Natural and Agricultural Sciences, University of Pretoria, Lynwood Road, Pretoria 0002, South Africa.

Keywords: Platinum group metals, acylthiourea, silica gel, adsorption, fixed-bed column, wastewater treatment, palladium recovery

The rising demand for platinum group metals (PGMs), particularly platinum (Pt) and palladium (Pd), alongside declining primary reserves, calls for efficient recovery strategies from secondary sources. This study presents the synthesis, characterization, and application of silica-anchored acylthiourea and amine adsorbents for selective Pt and Pd extraction from aqueous solutions that simulate industrial waste.

Two acylthiourea ligands, N,N-di(trimethoxysilylpropyl)-N′-benzoylthiourea (DTMSP-BT) and N-triethoxysilylpropyl-N′-benzoylthiourea (TESP-BT), were synthesized in high yields and covalently immobilized onto silica gel. Comparable amine-functionalized materials were prepared using bis(3-(trimethoxysilyl)propyl)amine (BTMSPA) and (3-aminopropyl)triethoxy silane (APTES). The resulting adsorbents were characterized using FT-IR, NMR, mass spectrometry, elemental analysis, XRF, PXRD, SEM, BET, and TGA-DTA. Ligand loadings ranged between 0.553 and 2.448 mmol per gram, and all materials exhibited thermal stability up to 600 °C.

Batch adsorption studies showed optimal Pt and Pd uptake at pH 2, with removal efficiencies exceeding 89 percent for the acylthiourea-functionalized adsorbents, even in the presence of competing metal ions. Adsorption capacity and selectivity followed the trend: DTMSP-BT-SG and TESP-BT-SG (highest), followed by APTES-SG, and then BTMSPA-SG. Fixed-bed column studies confirmed the potential for scale-up, with breakthrough capacities of 242.60 mg per gram for Pt and 194.29 mg per gram for Pd. Column mode outperformed batch mode due to longer contact times between the metals and the adsorbents. Desorption studies using thiourea-based eluents recovered up to 65 percent of the adsorbed metals, and the adsorbents remained structurally intact over five regeneration cycles.

This research highlights the superior performance of silica-anchored acylthioureas compared to more conventional amine-functionalized materials. Their high selectivity, capacity, and reusability make them promising candidates for sustainable recovery of critical PGMs from secondary sources such as industrial effluents.

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[2] WHO - Global Malaria Program, 1. Subregion GM. Status report on artemisinin resistance. 2014, **13**, 1–7.


L-PAL3
LECO
LECO

Exploring orthogonal ligand scaffolds for selective metal coordination

Werner E. van Zyl[a], *Welni Duminy,*[a] *Edmore Kangara*[a], *Nolwazi Mwelasi*[a]

[a]School of Agriculture and Science, Department of Chemistry, University of KwaZulu-Natal, Westville Campus, Durban, 4000 South Africa, Email: vanzylw@ukzn.ac.za

Keywords: orthogonal ligands, Group 11 metal complexes, synthesis, structures

We explored the concept of orthogonal ligands that were rationally designed to access high- and low-nuclearity Group 11 (Cu, Ag, Au) metal complexes. The aim was to prepare bifunctional ligands that contain both soft and hard donor atoms *on the same ligand unit* (orthogonal ligands) as they have the potential of providing different coordination modes to selectively synthesise heterometallic complexes. In particular, we focused on sulfur (soft) and nitrogen/oxygen (hard) donor atom sets. Although other soft/hard orthogonal ligand sets such as C/N, P/N, and P/O combinations to form heterometallic complexes are established [1], the S/N and S/O combination to form such complexes is rare.

The first example concerns the hierarchical self-organization of structurally complex high-nuclearity metal clusters with metallosupramolecular wheel architectures that are obtained from the self-assembly of smaller solvated cluster units, which is rare and unique. We used the heteroditopic monothiocarbonate ligand and demonstrated for the first time the synthesis and structure of a solvated non-cyclic hexadecanuclear cluster $[Cu\{SC(O)O^{i}Pr\}]_{16}\cdot 2THF$ that can simultaneously desolvate and self-assemble in solution and subsequently form a giant metallaring, $[Cu\{SC(O)O^{i}Pr\}]_{96}$. This cluster is the highest nuclearity copper(I) wheel and the largest metal cluster containing a heterodichalcogen (O, S) ligand reported to date [2]. The synthetic strategy described here opens new research avenues by replacing solvent molecules in stable $\{Cu_{16}\}$clusters with designed building units that can form new hybrid and multifunctional finite supramolecular materials. Subsequent work with the same ligand was also performed with silver(I) and gold(I), forming new complexes [3].

A second example concerns our recent work on cyaonooximes, in particular 2-oximino-2-cyano-thioacetamide (HTCO) [4] that contains a S donor (thione), N donor (cyano) and anionic O donor (oxime) on the same ligand, and its silver(I) complexes. We were able to describe a new silver(I)-TCO complex, and an X-ray crystal structure that showed a 1D coordination polymer, where the cyanoxime anion bridges through sulfur and oxygen [5].

This work will open new research avenues related to the properties and selectivity of these complexes.

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Metal-Organic Frameworks from Environmentally Benign Synthesis for Hydrogen and Carbon Dioxide Storage

Nejat Redwan Habib[a], *Isabel Diaz* [b], *Abi M. Taddesse* [c] *and Henrietta, W. Langmi*[a]

[a]Department of Chemistry, University of Pretoria, Private Bag X20, Hatfield, 0028, South Africa, E-mail: u25774400@tuks.co.za. [b]Instituto de Catálisis y Petroleoquímica, ICP-CSIC, C/Marie Curie 2, 28049 Madrid, Spain. [c]Department of Chemistry, Haramaya University, P.O. Box 138, Dire Dawa, Ethiopia.

Keywords: sustainable synthesis, metal-organic frameworks, hydrogen storage, CO_2 storage

Selected metal-organic frameworks (MOFs) including Al-MIL-53-NH_2, Fe-MIL-100, Zr-BDC and Zr-BDC-NH_2 were synthesized via a sustainable approach and tested for hydrogen and carbon dioxide storage. The synthesis was conducted at room temperature in the presence of water as a solvent [1]. Crystalline Fe-MIL-100, nanocrystalline Al-MIL-53-NH_2, and semi-crystalline Zr-BDC and Zr-BDC-NH_2 were formed as confirmed by powder X-ray diffraction. Thermogravimetric analysis shows that Zr-BDC was the most stable among the synthesized MOFs as it started to decompose above 500 °C. Morphological evaluation using field emission scanning electron microscopy reveals that Fe-MIL-100 consisted of octahedral-shaped crystals (Figure 1a) while Al-MIL-53-NH_2, Zr-BDC and Zr-BDC-NH_2 manifested as agglomerated particles. The agglomeration further validated by transmission electron microscopy, results from the clustering of nanocrystals or small particles (Figure 1b for Al-MIL-53-NH_2). This occurs due to the immediate formation of the precipitate during the room temperature in water synthesis for the specified MOFs. The highest Brunauer-Emmet-Teller (BET) surface area (2013 m^2/g), determined from nitrogen sorption, was recorded for Fe-MIL-100. Accordingly, Fe-MIL-100 exhibited the highest H_2 uptake (1.0 wt.% at 77 K and 1 bar, Figure 1c), and CO_2 storage (8.5 wt.% at 298 K and 1 bar, Figure 1d). This study illustrates the potential of certain sustainably produced MOFs for gas storage applications. Sustainably prepared MOFs provide the benefit of scalable synthesis suitable for industrial production by reducing reaction times and employing environmentally friendly solvents.

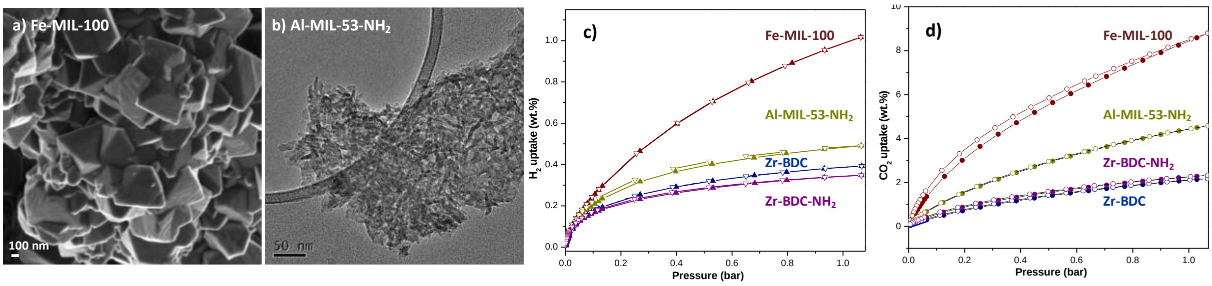

Figure 1 a) SEM micrograph of Fe-MIL-100, b) TEM image of Al-MIL-53-NH_2, c) H_2 isotherms at 77 K and d) CO_2 isotherms at 298 K for Al-MIL-53-NH_2, Fe-MIL-100, Zr-BDC and Zr-BDC-NH_2. Closed symbols are for adsorption and open symbols are desorption.

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Salicylaldehyde Cobalt–Schiff Base Complexes: Balancing Cytotoxicity and Albumin Pharmacodynamics for Next-Generation Therapeutics

Monika Nowakowska[a], *Ibrahim Waziri*[b], *Alfred J. Muller*[b], *Sheldon Sookai*[a]

[a]School of Chemistry, University of the Witwatersrand, PO WITS 2050, Johannesburg, South Africa, E-mail: Monika.nowakowska@wits.ac.za. [b]Research Centre for Synthesis and Catalysis, Department of Chemical Sciences, University of Johannesburg, Johannesburg, South Africa.

Keywords: Cobalt - Schiff base complexes, HSA, protein-ligand interactions, therapeutics

The incorporation of transition metals into bioactive organic ligands has emerged as a powerful strategy to modulate pharmacological profiles, enabling enhanced potency, refined selectivity, and novel modes of biological interaction. Within this framework, cobalt–Schiff base chelate complexes are particularly attractive, uniting cobalt's intrinsic biocompatibility, accessible redox states, and versatile coordination geometry. Nevertheless, the influence of such coordination chemistry on plasma protein transport, particularly interactions with human serum albumin (HSA), remains comparatively underexplored.

To address this, we designed, synthesised, and rigorously characterised a salicylaldehyde-derived Co(II) Schiff base complex (CoL) alongside the free ligand (HL) and selected transition-metal analogues for comparison. Structural elucidation by multimodal spectroscopic and analytical techniques, in conjunction with single-crystal X-ray diffraction, confirmed the targeted coordination architectures and solution stability.

Biological evaluation against MCF-7 breast adenocarcinoma cells revealed a pronounced potency enhancement upon cobalt coordination: HL displayed a modest IC_{50} of 39 μM, whereas CoL achieved sub-5 μM potency, with mechanistic evidence of a DNA-intercalative mode of action.[1] HSA-binding studies showed HL to have ~10-fold higher affinity ($\log K_a = 6.19$) than CoL ($\log K_a = 5.16$) at 310 K, indicating attenuated albumin association upon metal complexation. Thermodynamic analysis identified an entropy-driven, site-specific interaction at Sudlow's site I with minimal perturbation of secondary structure; near-UV circular dichroism, fluorescence quenching, molecular docking, and 100 ns molecular dynamics simulations corroborated localisation near Trp-214 and confirmed adduct stability.[2]

These findings reveal a functional duality with significant pharmacological implications: cobalt coordination markedly enhances cytotoxicity (CoL) by weakening HSA binding and increasing free drug availability, whereas the free ligand (HL) exhibits stronger HSA association that may limit immediate bioavailability yet prolong systemic circulation. This interplay between potency and pharmacokinetic behaviour emphasizes the need to optimise HSA affinity in metallodrug design. Salicylaldehyde-derived cobalt–Schiff chelates thus emerge as adaptable therapeutics scaffolds, where strategic ligand design, cobalt's coordination versatility, and controlled HSA-mediated transport together enable tunable stability, bioavailability, and tumour selectivity, thus laying the foundation for next-generation cobalt-based therapeutics.

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From Waste to Catalyst: Structural and Catalytic Evaluation of Coordination Polymers Synthesized from PET via One-Pot Mechanochemistry for Efficient Dye Removal from Water

Paula Maseko[a], Vincent J. Smith[b], Roderick B. Walker[c] and Theodore Geswindt[a]

[a] Department of Chemistry, Rhodes University, Cnr of University and Artillery Road, Grahamstown, 6139, South Africa E-mail: g22m0007@campus.ru.ac.za. [b] Department of Chemistry and Polymer Science, Stellenbosch University, de Beers building, Stellenbosch, 7600, South Africa. [c] Division of Pharmaceutics, Faculty of Pharmacy, Rhodes University, Makhanda, 6140, South Africa

Keywords: Metal-organic frameworks, PET upcycling, mechanochemical synthesis, methylene blue degradation, environmental remediation

Synthetic dyes such as methylene blue are persistent environmental contaminants that hinder light transmission in aquatic environments, interfere with photosynthetic processes, and exhibit toxic effects on aquatic life [1]. In this work, waste polyethylene terephthalate (PET) was upcycled through a one-pot mechanochemical approach to fabricate metal coordination polymers [2]. The process involved depolymerising PET into terephthalic acid and coordinating it with metals such as Zr, Co, Mn, and Zn. The as-synthesized 'coordination polymers' were characterized using powder X-ray diffraction (PXRD), Fourier-transform infrared spectroscopy (FTIR), and thermogravimetric analysis (TGA) [3,4]. The catalytic efficiency was assessed by degrading methylene blue at 25^{o} C under visible light, employing hydrogen peroxide as the oxidant. From our preliminary results, the Zr-based coordination polymer exhibits the highest degradation efficiency, achieving 80% dye removal within 3 hours. Reusability tests to evaluate catalytic stability over multiple cycles, are yet to be performed. This investigation underscores the potential of converting plastic waste into effective and recyclable catalysts for environmental clean-up applications.

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Ligand design strategies to optimize hydrogen production via Ru-catalyzed formic acid dehydrogenation

Andrew Swarts[a], Moegamat Joseph[a], Rotondwa Mphephu[a], Thabiso Mphuti[a], and Juliana Edor[b] Taylor[c]

[a] Swarts Research Group, School of Chemistry, University of the Witwatersrand, Braamfontein, 2050, South Africa, E-mail: andrew.swarts@wits.ac.za. [b]School of Physical and Chemical Sciences, North-West University, 1 Hoffman Street, Potchefstroom, 2520, South Africa

Keywords: ligand design, ruthenium, dehydrogenation, hydrogen production

Liquid Organic Hydrogen Carriers (LOHCs) have been identified as promising energy vectors necessary for the implementation of the hydrogen economy. These molecules undergo reversible hydrogenation and dehydrogenation cycles which enable hydrogen storage and release [1]. Formic acid (FA, HCOOH) is one of the most attractive LOHCs due to its favorable properties such as a high hydrogen content (4.4 wt%) and a high energy density (1.77 kWh/L) [2]. In our group we have developed three ruthenium(II) catalyst families bearing different ligands: i) pyrazolyl-pyridine [3], pyridyl-formamidine [4], and iminopyridine [5], which were evaluated for hydrogen production via formic acid dehydrogenation. This talk will rationalize structure-activity relationships and differences as influenced by ligand steric and electronic properties. Also, insights gained from mechanistic studies will be delineated to contribute to rational catalyst design strategies.

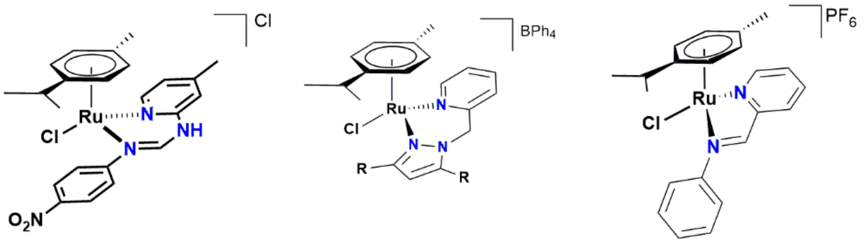

Fig. 1 High-performance hydrogen production catalysts produced in the Swarts Research Group.

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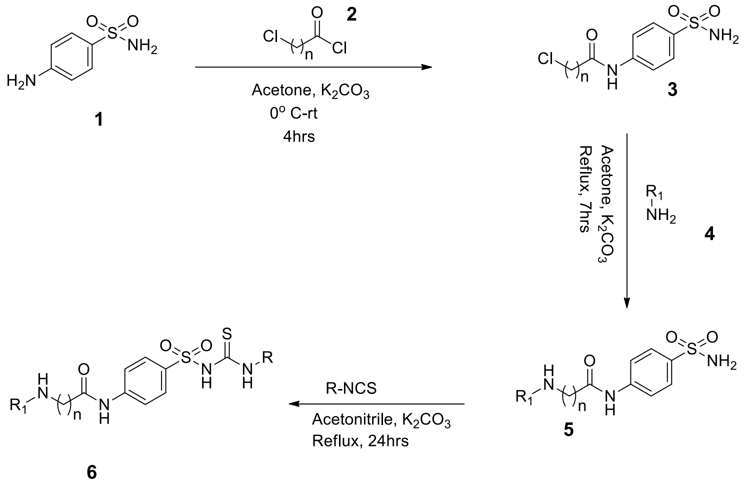
Synthesis of Sulfonylthioureas as Potential Antidiabetic Drugs

Tiyisela N Mbhokazi, Mpelegeng V Bvumbi and Simon Mnyakeni Moleele

[a] Department of Chemistry, Faculty of Science, Engineering and Agriculture, University of Venda, Thohoyandou, Limpopo Province, South Africa; Email address: mnyakeni.moleele@univen.ac.za

Keywords: Diabetes, Sulfonylthioureas, Alpha Glucosidase, Alpha Amylase

Diabetes is a metabolic disease that occurs when there is a deficiency in insulin production or no insulin in the pancreas.[1] It is estimated that the number of people affected by diabetes will rise to 700 million by 2045, leading the World Health Organization to consider diabetes an epidemic.[2] Diabetes imposes a significant financial burden on the public healthcare in South Africa and the world at large. The purpose of this project was to synthesize a series of sulfonylthioureas as antidiabetic drugs by converting a urea to thiourea moiety. The novel sulfonylthioureas were designed and synthesized over three reaction steps using different appropriate synthetic methods (**Scheme 1**). The successfully synthesized final compounds were probed for their antidiabetic activity against alpha-glucosidase and alpha-amylase.



where R= phenyl,cyclohexyl,butyl,propyl
R_1= Morpholine, Aniline, N-Methylaniline, 2,6-N-Methylaniline
n = 1 or 2

Scheme 1: Synthetic scheme

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Development of norbornene-based compounds as MAO-B inhibitors for the treatment of Parkinon's Disease

Bridget Mtetwa[a], Dr. Ayodeji Egunlusa[a] and Prof. David S. Khanye

[a] Department of Pharmaceutical Chemistry, Rhodes University, Drodsty Road, Grahamstoen, 6139, South Africa, E-mail: g18m2417@campus.ru.ac.za

Keywords: Parkinson's disease, norbornene, MAO-B inhibition, antioxidants, neuroprotection, imides

Purpose:

Parkinson's disease (PD) is the second most common neurodegenerative disorder of the central nervous system, characterised by the progressive degeneration and impaired function of dopaminergic neurons in the substantia nigra, pars compacta [1]. A contributing factor to this loss of function is the excessive metabolism of dopamine by the monoamine oxidase-B (MAO-B) enzyme, which promotes oxidative stress and further exacerbates neuronal degeneration and dysfunction. Clinically, PD presents with motor symptoms—such as bradykinesia, resting tremors, rigidity, and postural instability—as well as non-motor symptoms like cognitive decline, sleep disturbances, and depression [2]. Current treatments only offer symptomatic relief but do not halt disease progression. A good example is the MAO-B inhibitors like selegiline and rasagiline, which reduce dopamine breakdown. However, prolonged use has been linked to adverse effects such as worsened dyskinesia, nausea and hallucinations [3]. Therefore, there is an urgent need for therapies that preserve dopamine while offering neuroprotection. This study aims to design, synthesise, and characterise a series of norbornane-based compounds as MAO-B inhibitors with potential antioxidant activity. Norbornane scaffolds provide structural rigidity and metabolic stability, supporting their potential as dual-action agents for the safer and more effective treatment of PD.

Methods:

Norbornene-derived scaffolds were developed using in silico drug design. Cycloaddition reaction yielded cis-5-norbornene-endo-2,3-dicarboxylic anhydride, which was derivatised under reflux conditions to afford the final product. Products were purified by either by recrystallisation or chromatography method, and the structures were confirmed using ^{1}H, ^{13}C NMR and mass spectroscopy.

Results:

Norbornene-derived imide compounds were successfully synthesised in yields ranging from 42% to 72%, and the structures were confirmed via NMR spectroscopy. Molecular docking studies against MAO-B revealed binding energies between –8.1 and –10.0 kcal/mol for all compounds, when compared to safinamide (–12.136 kcal/mol). Investigation of the binding site suggests strong and favourable interactions within the active site. All synthesised compounds satisfied Lipinski's Rule of Five, supporting their drug-likeness and potential for oral bioavailability. In silico ADME studies predict favourable blood-brain barrier permeability.

Conclusion:

Preliminary results indicate that norbornene-based derivatives are promising candidates for MAO-B inhibition, exhibiting favourable binding affinity, drug-like properties, and blood–brain barrier permeability. Ongoing studies, including biological evaluation, antioxidant assays, and cytotoxicity profiling, are essential to fully establish their therapeutic potential or determine the need for further optimisation.

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Synthesis, characterization and cytotoxicity of aminothiazole chiff and metal complexes

Temitope E. Olalekan[a], *Horacio López-Sandoval*[b] *and Nórah Barba-Behrens*[b]

[a]Department of Chemistry, University of Ibadan, Ibadan 200285, Nigeria, E-mail: topeolalekan11@yahoo.com.
[b]Departmento de Química Inorgánica, Universidad Nacional Autónoma de México, C.U., Coyoacán 04510, Ciudad de México, México

Keywords: Schiff base, aminothiazole, metal complexes, cytotoxicity, IC_{50}, LD_{50}

A thiazole-derived ligand, tzpH, and the coordination compounds with Mn(II) Co(II), Ni(II), Cu(II), Zn(II), Pd(II), and Ag(I) were synthesized and characterized by elemental analysis, ^{1}H and ^{13}C NMR, FTIR, UV-Vis, mass spectra, and magnetic susceptibility measurements. ^{1}H NMR spectra of the Zn(II) complex indicated the ligand coordinated to the zinc ion through the phenolate oxygen ion, due to the absence of the O–H signal, however in the in the case of the [Ag(tzp)NO_3], the phenolate oxygen proton was observed.

The infrared spectra of the coordination compounds allowed the assignment of the monodentate, bidentate or tridentate coordination mode of the ligand in each metal center, based on the vibrational frequencies of the azomethine *v*(C=N), thiazoline *v*(C=N) and *v*(C–O). The elemental CHNS and the mass spectra of the compounds were consistent with the assigned molecular formulas. The reflectance electronic spectra of the Co(II), Ni(II) and Cu(II) compounds showed tetrahedral or octahedral geometries for the metal ions. The magnetic moments of Co(II), Ni(II), Cu(II) complexes were indicative of high spin states while Zn(II) and Ag(I) complexes were diamagnetic.

The cytotoxicity of the derived compounds was investigated on breast, cervical, prostrate and colon cancer cell lines and mouse fibroblast. The silver(I) complex, [Ag(tzp)NO_3], was shown to be most active with higher IC_{50} values of 10.5 µg/mL (HeLa) and 1.46 µg/mL (HCT-15) than *cis*-platin. The lethal dose, LD_{50} at 26.19 mg/kg indicated the viability of the therapeutic use of [Ag(tzp)NO_3] against cervical and colon cancers. Further investigations including animal studies are being carried out.

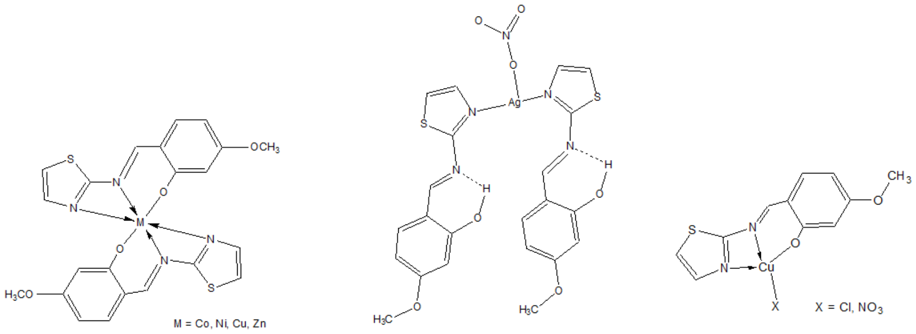

Figure 1. Formulas of Cu(II), Pd(II) and Ag(I) complexes of tzpH.

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Leveraging Quantum Mechanical and Machine Learning technologies for predictive modelling of Soursop (Annona muricata Linn.) Phytochemical Extracts Against Breast Cancer

Vitalis Mbayo[a], *Penny P. Govender*[a], *Vincent A. Obakachi*[a], *and Krishna K. Govender*[a]

[a]Department of Chemical Sciences, Faculty of Science, University of Johannesburg, Johannesburg, 2094, South Africa.
E-mail: vmbayo92@gmail.com.

Keywords: Machine learning, quantum chemistry, Computational Chemistry, breast cancer, Soursop (Annona muricata Linn).

Breast cancer is a major health concern for women in sub-Saharan Africa, with cases in South Africa doubling and now representing 14–30% of female cancers. The five-year survival rate is under 50%, but improvements could be made by addressing treatment and diagnostic gaps, along with developing targeted chemotherapies to reduce side effects [1] [2]. A multitargeted drug design strategy is proposed to address breast cancer by developing a single medication that targets interconnected proteins and pathways, as current treatments for advanced stages are ineffective against metastasis [3] . Natural products (NPs) play a crucial role in drug discovery, with 3.8% of approved drugs being unaltered NPs and 18.9% as NP derivatives from 1981 to 2019 [4]. Notable examples include Taxol and Vinblastine, both used in cancer treatment. African natural product databases present valuable, unscreened compounds for breast cancer research. Given the traditional drug discovery process's high costs and duration, computational methods are promising for identifying new anti-cancer agents [5]. GaussView will be utilised to calculate geometry optimisation with Density functional theory, M062X functional and def2svp basis set [6]. We virtually screened 52,542 Soursop phytochemicals against the key cancer target Cyclooxygenase-2 (COX-2), an enzyme that promotes tumour growth, in our objective to find effective inhibitors. After performing Molecular Docking, further virtual screening and Molecular dynamics simulation calculations, five compounds demonstrated reasonable potential therapeutic effects compared to 2 control Food and Drug (FDA) approved drugs currently on the market. Reducing the expression of the COX-2 enzyme may help slow the progression of cancer. In this study, we aim to identify novel, drug-like natural product inhibitors from Annona muricata for breast cancer treatment and to discover similar lead compounds from selected African natural product databases using advanced virtual screening and computational chemistry methods.

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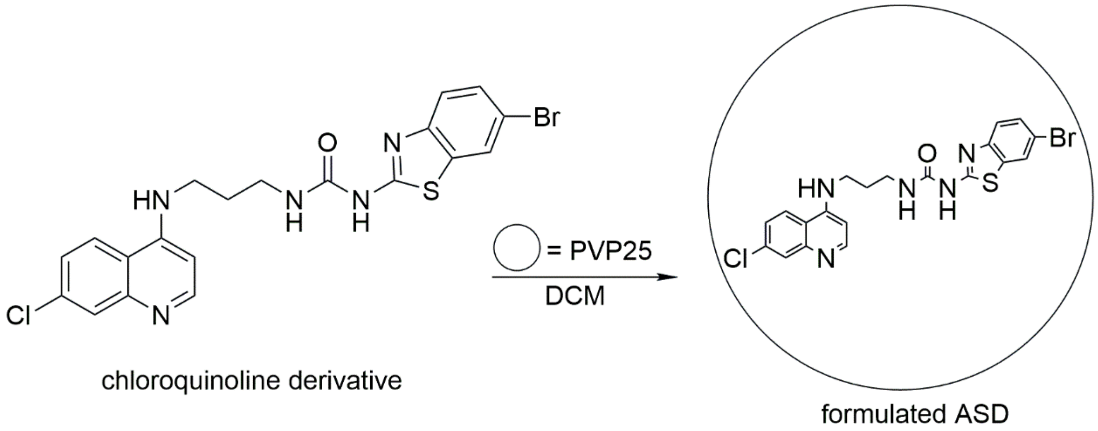
The formulation of a novel chloroquinoline derivative in an amorphous solid dispersion and the determination of its thermal and solubility parameters

Thrineshen Moodley[a]*, Nikhail Raghunundhan*[b] *and Wilna Liebenberg*[a]

[a] Department of Chemistry, Faculty of Science, Engineering and Agriculture, University of Venda, Thohoyandou, 0950.
E- [a]NWU Preclinical Drug Development Platform, North-West University, Potchefstroom, , South Africa, E-mail: Thrineshen.Moodley@nwu.ac.za

Keywords: Pharmaceutics, DSC, Solid State Chemistry, XRD

This study aimed to improve the solubility of a novel chloroquinoline derivative by developing an amorphous solid dispersion (ASD) drug delivery system using polyvinylpyrrolidone (PVP K25) as a polymeric carrier. The ASD was prepared by mixing the test compound with PVP-K25 in the presence of dichloromethane followed by rotary evaporation and vacuum drying at 60°C for 24 h. The resulting formulation was characterised by Differential Scanning Calorimetry (DSC), Modulated DSC (MDSC), X-ray Powder Diffraction (XRPD), and Polarised Light Microscopy (PLM). A glass transition (*T*g) of 136.98°C was confirmed. XRPD analysis showed reduced crystallinity further confirmed by traces of crystallinity in PLM. Solubility and dissolution studies were conducted and analysed by UV spectroscopy. The results showed a significant increase in chloroquinoline derivative concentrations within the ASD formulation compared to the unformulated chloroquinoline derivative. These findings suggested that the ASD formulation is a promising approach to enhance the solubility and potentially improve the bioavailability of the chloroquinoline derivative in future *in vivo* studies.



Nucleophilic reactions of cyclobutenones

Sarah Wright and *Songeziwe Ntsimango*

[a] Department of Chemistry, University of the Witwatersrand, Braamfontein, Johannesburg, 2000, South Africa. E-mail: 1849458@students.wits.ac.za.

Keywords: cyclobutenone, nucleophilic reactions, ring opening, ring rearrangement

Cyclobutenones are key intermediates to various reactions, with a large ring strain that makes them susceptible to strain-release reactions [1-2]. They are versatile building blocks in organic and medicinal chemistry and can be included in complex molecules under mild reaction conditions [2]. Due to their conjugated enone moiety, cyclobutenones can undergo multiple reactions, including Michael addition reactions that can result in ring rearrangement as well as ring opening reactions [1]. This study looks at the nucleophilic reactions of silylated cyclobutenones under acidic and alkaline reaction conditions. In addition, mechanistic studies, scope and limitation of the reactions were also examined. As shown in Figure 1, when cyclobutenone **1** reacts with TBAF and acetic acid, the acetic acid adds onto the ring to form compound **2**, in a ring rearrangement reaction, where the nucleophile attaches at the 3-position, with some of the cyclobutenone only undergoing desilylation to form **3**. When **1** is reacted in K_2CO_3 and methanol, the methanol attaches onto the ring, causing a ring opening in the 1,2-addition reaction to generate compound **4**.

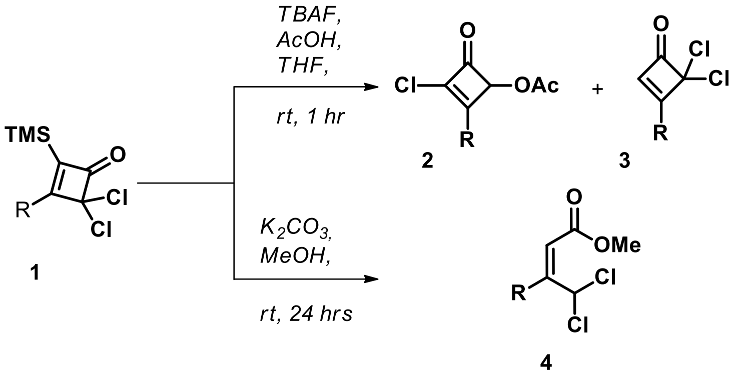


Figure 1. A general scheme of the nucleophilic addition reactions that occur on the TMS-cylobutenone ring during various desilylation reactions.

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In Search of the Resurrection Plant Metabolite 3,4,5-tri-*O*-galloylquinic

Marwaan Rylands

[a] Department of Chemistry, University of Cape Town, Rondebosch, Cape Town, 7700, South Africa
E-mail: marwaan.rylands@uct.ac.za

Keywords: plant metabolites, natural products, polyphenols

Myrothamnus flabellifolius (*M. flabellifolius*), a well-known resurrection plant, has been widely studied for its varying medicinal properties as well as its high desiccation tolerance.[1] It is distributed across areas of Namibia, Botswana, Zimbabwe and South Africa and there are several review articles that highlight the importance of this plant in traditional medicine and its therapeutic potential.[1-4] One of the major compounds found in *M. flabellifolius* is 3,4,5-tri-*O*-galloylquinic acid, which was identified as the predominant polyphenol accounting for 74% of the total mass of dehydrated leaves.[5] Both resurrection plant extracts and the isolated 3,4,5-tri-*O*-galloylquinic acid have shown a variety of interesting biological activities.[6-8] As a result, there has been a growing interest in access to 3,4,5-tri-*O*-galloylquinic acid, to further probe the focus of the plant's medicinal properties and to explore the application of this interesting polyphenol. In this talk, I will share our attempts at isolating and quantifying 3,4,5-tri-*O*-galloylquinic acid in *M. flabellifolius* leaves. I will also report on our recent total synthesis of 3,4,5-tri-*O*-galloylquinic acid, employing a modified Steglich esterification as a key step, as well as some of the preliminary antioxidant and wound healing data for both extracts and the synthesized compound. Finally, I will discuss in the context of this project and perhaps more generally, the complementarity of isolative- and synthetic chemistry in natural products.

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Effects of structural modification on established BODIPY dye properties for modern applications

Aviwe May[a,b*], *Bokolombe P. Ngoy*[c], *John Mack*[a], *Tebello Nyokong*[a]

[a]Institute for Nanotechnology Innovation, Rhodes University, Makhanda 6140, South Africa.
[b]Chemical Resource Beneficiation, North-West University, Potchefstroom 2520, South Africa. E-mail: Aviwe.May@nwu.ac.za.
[b]Département de Chimie, Université de Kinshasa, Kinshasa, Democratic Republic of the Congo South Africa

Keywords: BODIPY, quantum yield, fluorescence, optical limiting, singlet oxygen, PACT

Boron-dipyrromethene (4,4-difluoro-4-bora-3a,4a-diaza-s-indacene or BODIPY) dyes are structural analogues of porphyrins. BODIPYs have been significantly researched over the past few decades, and because they possess favourable properties, they have a wide range of potential applications that are a subject of ongoing research [1–2]. These properties include a facile synthesis & structural versatility, excellent spectroscopic properties (e.g. narrow Gaussian-shaped absorption and emission bands), high molar extinction coefficients, high fluorescence quantum yields & negligible triplet-state formation and sensitivity to solvent polarity, and high solubility in commonly used organic solvents of differing polarities [1]. The structural versatility of BODIPYs allows the introduction of various functional groups around the BODIPY core (Figure 1). This structural modification leads to desirable structure-property relationships, and has been successfully demonstrated with a series of previously synthesised dyes with respect to fluorescence properties, optical limiting (OL) properties and singlet oxygen properties & Photodynamic Antimicrobial Chemotherapy (PACT) activity [3–6]. The introduction of different substituents at the *meso*-position or α- and β-positions enhances or decreases the fluorescence quantum yield of the dyes, depending on the position on which the heavy atoms are introduced. A decrease in fluorescence due to the presence of heavy atoms has a direct correlation with an increase in the singlet oxygen quantum yield, although it does not necessarily lead to better PACT activity. On the OL front, the introduction of styryl groups at the 3,5-positions can lead to the formation of BODIPYs with strong donor-π-acceptor (D-π-A) properties and favourable optical limiting properties [4]. Current and future research & applications of structurally modified BODIPYs will also be described.

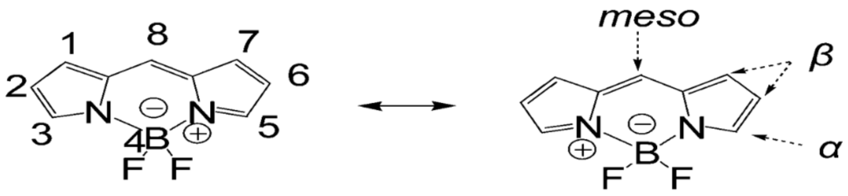

Figure 1 The numbering system of the structurally versatile BODIPY core.

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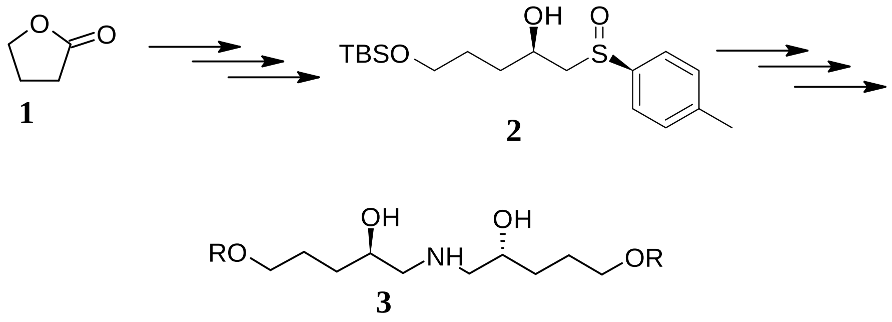
Towards the synthesis of hydroxylated polyamines

Memory Zimuwandeyi[a], Amanda L. Rousseau[a], Moira L Bode[a]

[a]Address University of the Witwatersrand 1 Jan Smuts Avenue, Johannesburg, E-mail: memory.zimuwandeyi@wits.ac.za

Keywords: Polyamines, sulfoxide.

Polyamines are described as aliphatic organic compounds with two or more primary amine substituents, connected by one or more methylene linkages within their structure.[1] Biological properties exhibited by this class of compounds has seen them being incorporated into different chemotherapeutic strategies for various diseases as either drug vectors or therapeutic agents. Interestingly, substitution of the methylene linkage of polyamines is not commonly observed in the naturally occurring substrates. Identification and characterisation of a polyamine toxin, pavettamine, with a five-carbon linker having a 1,3-*syn*-diol functionality piqued our interest and led us to develop methodologies for synthesising reduced functional analogues of this unusual compound.[2] A synthetic route towards the hydroxylated polyamines starting from commercially available small molecules like γ-butyrolactone **1**(**Scheme1**) will be discussed. The sulfoxide chiral auxiliary was employed for stereochemical control and this approach afforded intermediate **2** which was further transformed yielding precursor polyamine **2**.



Scheme 1: Synthetic approach to hydroxylated polyamines

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The role of dipicolinic acid in enabling the simultaneous voltammetric analysis of copper and bismuth.

Masego Ramonyai *and Caren Billing*

[a] School of Chemistry, University of the Witwatersrand, 1 Jan Smuts Ave, Braamfontein, Johannesburg South Africa
E-mail: 0719016m@students.wits.ac.za

Keywords: Bismuth, Copper, Interfering ions, Dipicolinic acid, Voltammetry.

In environmental samples a range of metal ions are often found in a single sample. In the interest of analyzing low concentrations of bismuth in environmental samples by voltammetric methods, the presence of interfering ions must be considered. It has been shown that the voltammetric response for Cu(II) and Bi(III) greatly overlap, making it impossible for the direct analysis of these metal ions together using techniques such as anodic stripping voltammetry (ASV).[1,2] In an effort to separate the overlapping peaks, the introduction of a chelating ligand such as dipicolinic acid (DPA) was investigated. It is known that the reduction of ML complexes occur at more negative potentials than that of uncomplexed M.[3] Bi(III) and Cu(II) form stable complexes with dipicolinic acid across a wide pH range, but importantly, the addition of DPA successfully separates the bismuth and copper peaks. This study was done at very low pH (~0.3) where the diffusion junction potential is extensive due to the high H^+ concentration but where complications due to hydrolysis can be avoided.[4] It was demonstrated in some preliminary studies that the addition of dipicolinic acid (DPA) as a complexing agent delays the hydrolysis of Bi(III). Experiments were conducted at bismuth and copper concentrations in the μM range and ~300 times excess of DPA and evidently, Cu-DPA and Bi-DPA species form successfully at the pH studied. Increasing the concentration of Cu(II) in solution did not affect the stability of the Bi-DPA complexes or the peak current for bismuth. Moreover, an increase in Bi(III) concentration in solution led to a linear increase in the bismuth peak current. It was thus concluded that excess presence of DPA in solution resolves the bismuth copper peaks and anodic stripping voltammetry (ASV) is a suitable voltammetric technique for these measurements.

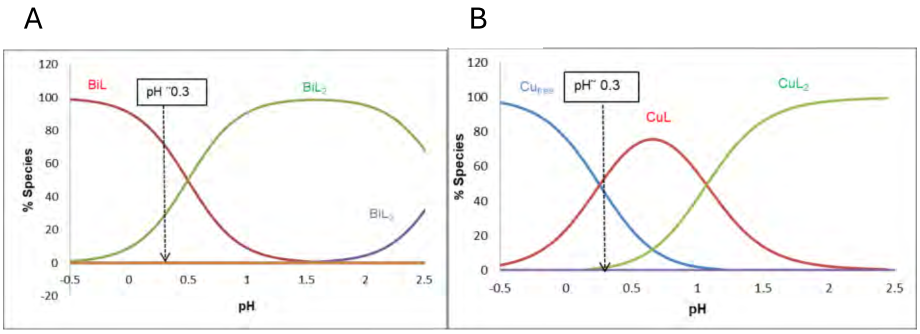

Figure 1: Species distribution diagram (SSD) for A) Bi(III) and B) Cu(II) in DPA with ratio 1:300.

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CQD-TiO_2 composite as a potential crypto-electrode modifier for high-performance aptasensing with ultra-low detection limits

Indiphile Nompetsheni[1], *Xolile Fuku*[1], *Ntuthuko Wonderboy Hlongwa*[1], *Nithyadharsen Palaniyandy*[2]

[a1]Institute for Nanotechnology and Water Sustainability (iNanoWS), College of Science, Engineering, and Technology, University of South Africa, Roodepoort, Florida, 1710, South Africa
[2]Institute for catalyst and Energy Sustainability (ICES), College of Science, Engineering, and Technology, University of South Africa, Roodepoort, Florida, 1710, South Africa
Email: 21068046@mylife.unisa.ac.za, fukuxg@unisa.ac.za

Keywords: Aptasensor, CQD–TiO_2 composite, *Cryptosporidium*, Water

Cryptosporidium is the parasite that has emerged as a major cause of diarrheal illness. Its presence in water bodies poses a significant treat to immunosuppressed individuals, young children, even healthy adults. Therefore, it is crucial to monitor this pathogen to prevent such outbreaks. This paper highlights the formation of carbon quantum dot-titanium dioxide nanoparticles (CQD–TiO_2) composite, specifically designed for electrochemical sensing of Cryptosporidium. The composite material was prepared by combining CQD with TiO_2, to improve the electrochemical characteristics of CQD. The characteristics of the CQD–TiO_2 composite were evaluated using a variety of characterization techniques, such as X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDS), Raman spectroscopy, high resolution Transmission electron microscopy (HR-TEM), Fourier transform infrared (FTIR) confirmed the successful incorporation of TiO_2 showing a uniform dispersion of CQD which highlighted the existence of titanium, carbon, and oxygen in the composite. The electrochemical characteristics of the CQD–TiO_2 composite were studied using Electrochemical impendence spectroscopy (EIS), and cyclic voltammetry (CV) revealing an enhanced charge transfer rate and improved electrochemical stability compared to pure TiO_2. The CQD–TiO_2 composite was used as an electrode modifier to fabricate an electrochemical aptasensor. The aptasensor demonstrated a good performance, achieving a limit of detection (LOD) of 0.0024 µM within a linear concentration range of 0.0025–0.0045 nM, making it highly suitable for a variety of applications related to sensing. The aptasensor showed a high sensitivity of 0.2706 mA/ nM, which is notably high for trace of *Cryptosporidium*.

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Synthesis and characterization of mono, bi and tri composite of Ag, ZnO and MWCNT modified SPC electrode.

Kabelo S. Banda, and Omolola E. Fayemi

[a] Department of Chemistry, School of Physical and Chemical Sciences, Faculty of Natural and Agricultural Sciences, North-West University (Mafikeng Campus), Private Bag X2046, Mmabatho, 2735, South Africa. Material Science Innovation and Modelling (MaSIM) Research Focus Area, Faculty of Natural and Agricultural Sciences, North-West University (Mafikeng Campus), Private Bag X2046, Mmabatho, 2735, South Africa. E-mail: kabelobanda11@gmail.com

Keywords: Cyclic voltammetry, mono, bi, tri, multi-walled carbon nanotube, screen printed carbon electrode

The bare surface of screen-printed electrodes has been improved overtime with the process of dropped-dry or electrodeposition modification with nanomaterials. The nanomaterials explored in the study are Zinc Oxide (ZnO) and Silver (Ag) nanoparticles, fMWCNTs. The nanomaterials namely Zinc Oxide (ZnO) and Silver (Ag) nanoparticles, fMWCNTs, the single material mono modification were compared with the bi-composites fMWCNTs/Ag, fMWCNTs/ZnO, and tri-composite fMWCNTs/Ag/ZnO were characterized by using fourier-transform infrared spectroscopy (FT-IR), x-ray diffraction spectroscopy (XRD), energy dispersive x-ray spectroscopy (EDS), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The electrochemical properties of the bare and modified SPC electrodes were investigated by using cyclic voltammetry. The investigation showed that the tri-composite SPC/fMWCNT/ZnO/Ag showed improved catalytic properties and current response than the SPC/fMWCNT, SPC/ZnO, SPC/Ag, the bi-composites of SPC/fMWCNT/ZnO and SPC/fMWCNT/Ag. Further investigation also revealed the reaction at the surface of the electrodes and kinetics of electron transfer process.

A Comparative Material-Performance Study of Sulphur-and Phosphorous-Doped Reduced Graphene Oxides for Electrochemical Biosensing of Organophosphorus Pesticides

Ijimdiya, Racheal Ukachi[a,b]; *Olatunji, Stephen Olatunde*[a]

[a]Department of Chemistry, School of Chemistry and Physics, University of KwaZulu-Natal, South Africa
[b]Department of Chemical Science, Faculty of Sciences, Anchor University, Lagos, Nigeria
224196168@stu.ukzn.ac.za

Keywords: lectrochemical biosensors; Food safety; Environmental monitoring; Nanomaterials; Real-time detection

Electrochemical biosensors are at the pole position of analytical innovation, presenting quick, ultra-sensitive recognition of environmental pollutants like pesticides, to safeguard food and public health. This study presents a comparative analysis of sulfur-and phosphorus-doped reduced graphene oxides (S-rGO and P-rGO) as future transducer materials for electrochemical biosensing. Graphene oxide (GO) was synthesized through a modified Hummer's method and afterwards doped and reduced using sodium disulfide (NaS_2) for S-rGO and triphenylphosphine (TPP) for P-rGO, respectively. Characterizations were carried out using advanced spectroscopic and electrochemical techniques. Results revealed that doping considerably modulates the physicochemical properties of rGO, X-ray diffraction confirmed amorphous structures with interlayer reordering after doping. FTIR results indicated considerable removal of oxygen containing functional groups in both S-rGO and P-rGO, UV-Vis spectroscopy indicated band gaps of 2.85eV for S-rGO and 2.59eV for P-rGO, while photoluminescence data suggested a higher defect density in S-rGO at 430 λ. Thermal analysis revealed improved thermal stability for S-rGO (608 ^oC) compared to P-rGO (563.5 ^oC). BET confirmed larger surface area and pore volume of SrGO (204 m^2/g, 0.0621cm^3/g vs 158 m^2/g, 0.11 cm^3/g). Electrochemical profiling established the superiority of S-rGO, exhibiting a larger electroactive surface area (260.88 cm^2 vs. 86.58 cm^2) and lower electron transfer resistance of 35 Ω and 64 Ω for S-rGO and P-rGO respectively. Cooperatively, these results point to the critical role of heteroatom doping in modifying graphene-based materials for analytical performance. S-rGO, with its higher thermal, electronic, and structural properties, appears as a highly potential material for the sensitive detection of organophosphorus pesticides. This work gives valuable insights into materials-driven developments for biosensor technology, with important suggestions for environmental monitoring and food safety assurance.

Carbonization of Hemp-Derived Carbons: A Comparative Study of Activation Routes

Funmilola Adesanya, Ernst Ferg and Xandri van Niekerk

[a] Department of Chemistry and uYilo e-Mobility Programme, Nelson Mandela University, P.O.Box 77000, Port Elizabeth 6031, South Africa. E-mail: s232272468@mandela.ac.za, Ernst.Ferg@mandela.ac.za.

Keywords: hemp-derived carbon, chemical activation, Cannabis sativa L., sustainable, sodium-ion battery

The quest for sustainable, affordable energy storage keeps sodium-ion batteries at the forefront of battery research, especially for large-scale applications where lithium-ion systems are costly. Industrial hemp (Cannabis sativa L.), a rich lignocellulosic, low-cost biomass, holds huge promise as a sustainable carbon precursor for diverse applications, even as anode materials in energy storage devices like sodium-ion batteries. Optimizing the structural properties and electrochemical performance of this carbon, however, remains challenging. In this study, the carbonization and activation of hemp cores and fines will be carried out in a single step using four commonly utilized chemical activators: potassium hydroxide (KOH), zinc chloride ($ZnCl_2$), potassium carbonate (K_2CO_3), and phosphoric acid (H_3PO_4). The effects of each chemical activator on the microstructural and textural properties of the hemp-derived carbon will be evaluated by means of analytical techniques such as scanning electron microscopy (SEM), Brunauer-Emmett-Teller (BET) surface area analysis, powder X-ray diffraction (PXRD), energy-dispersive X-ray spectroscopy (EDS), and thermogravimetric analysis (TGA). Also, the electrochemical performance will be assessed in sodium-ion battery half-cells. The findings of the study are anticipated to show the impact of different activation chemistries on the properties of the synthesized carbons and offer insights for optimizing hemp-derived carbons for energy storage applications.

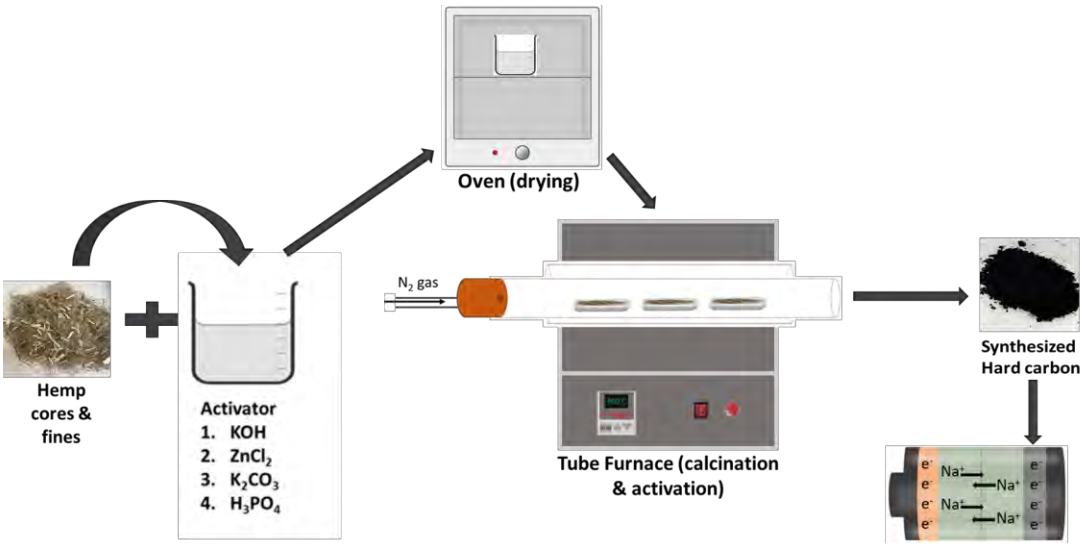


Figure 3: Schematic representation of the calcination and activation process to obtain hemp-derived carbon

Effect of pyrolysis temperature of *Kigelia africana* biochar for the adsorption of lead(II) ions from aqueous solution

Nomaswazi C. Madonsela, Bice S. Martincigh, Vincent O. Nyamori, and Bhekumuzi P. Gumbi

[a] School of agriculture and Science, University of KwaZulu-Natal, Westville Campus, Durban, 4000, South Africa, Email: 213539701@stu.ukzn.ac.za

Keywords: adsorption, lead, biochar, pyrolysis

Recently, the focus of water pollution remediation has shifted towards developing environmentally friendly adsorbents with robust stability. *Kigelia africana* fruit has been identified as an effective and low-cost precursor for potential adsorbents for removing heavy metal ions from aqueous solutions. Lead is one of the most hazardous environmental pollutants due to its high toxicity, tendency to accumulate in the biosphere, and persistence, making it difficult to remove from effluent by traditional water treatment plants, causing ecological imbalance. Therefore, the use of advanced materials and technologies to eliminate these pollutants from wastewater is crucial for maintaining a safer environment. This study aimed to make biochar from *Kigelia africana* fruit and to investigate its potential capacity for removing Pb^{2+} from water. The biochar from *Kigelia africana* was synthesized through pyrolysis at different temperatures (400 - 800 °C). Batch adsorption experiments were performed to determine the effects of initial pH, biochar dose, adsorption time, temperature, and initial Pb^{2+} concentration. The results showed that increasing the pyrolysis temperature improved the adsorption efficiency and capacity. The adsorption of Pb^{2+} onto *Kigelia africana* biochar (KAB) prepared at different temperatures of the biochar (KAB-400, KAB-500, KAB-600, KAB-700, and KAB-800) gave Langmuir maximum adsorption capacity (q_{max}) values of 21.01, 25.12, 27.38, 32.47, and 46.09 mg $g^{-1,}$ respectively. The Elovich kinetics model fitted the data best. The equilibrium data were best explained by the Fruendlich (for KAB-400), Langmuir (for KAB-500 and KAB-600), and Sips (for KAB-700 and KAB-800) isotherm models. In conclusion, these results illustrate that the biochar produced from *Kigelia africana* fruit could play a role in environmental pollution mitigation by enhancing the removal of Pb^{2+} from conventional wastewater treatment effluent, thereby minimizing its potential risks to the environment.

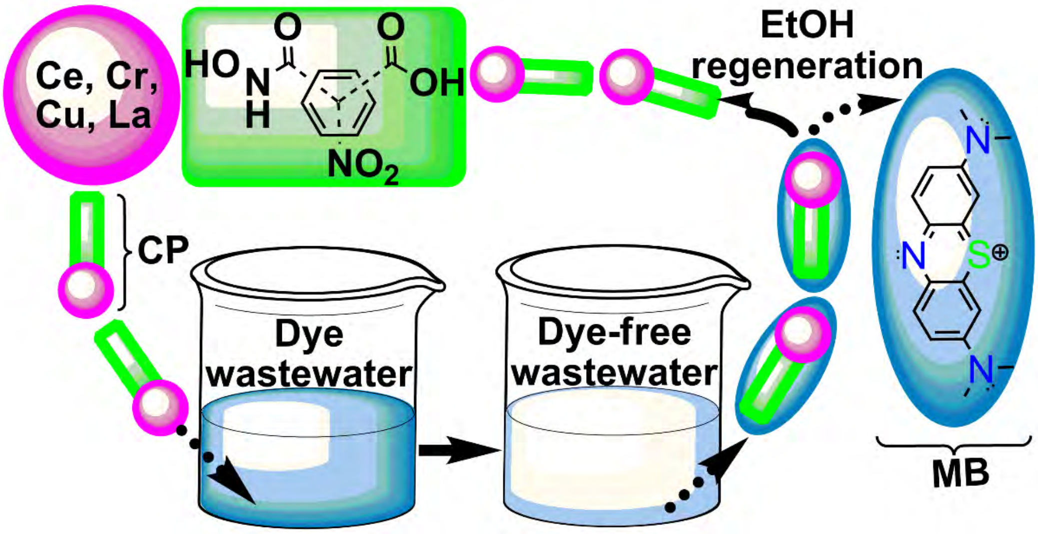
Investigating the efficiency of transition and lanthanide-metal based coordination polymers for methylene blue adsorption

Cresten Moodley[a], *Alfred Muller*[a]

[a] University of Johannesburg, Department of Chemical Sciences, P.O. Box 524, Auckland Park, 2006, South Africa. Email: crestenm464@gmail.com.

Keywords: Adsorption, adsorbent, coordination polymer, methylene blue, solvothermal

Global water systems face mounting pollution pressures from industrial effluents, especially dye-rich wastewater from leather, paper and textile sectors [1]. Conventional biological, chemical and physical dye removal strategies are typically limited in efficiency, sustainability or scalability [2]. Among physical methods, adsorption stands out for its simplicity and minimal chemical requirements, but traditional adsorbents like activated carbon and zeolites face challenges in regeneration and selectivity [3]. However, coordination polymers (CPs) constructed from metal ions and organic linkers could offer a promising alternative due to their tunable porosity, high surface area and post-synthetic modifiability [4]. This study reports the synthesis of 12 CPs using three linkers (benzene-1,4-dicarboxylic acid (BDC), benzene-1,4-dihydroxamic acid (BHA), 5-nitroisophthalic acid (5NIP)) coordinated with La, Ce, Cu and Cr ions. These metals were selected for their stability, coordination behavior and cost-effectiveness. The resulting CPs were evaluated for the adsorption of methylene blue (MB), a model dye pollutant. The study emphasizes enhancing aqueous stability, adsorption efficiency and minimizing metal leaching, thereby contributing to the development of robust, recyclable materials for sustainable wastewater remediation.



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Organobentonite–Ag/TiO₂ Composite for Cr(VI) Removal and Bacterial Disinfection

Dipuo P. Kgabi *and Abayneh A. Ambushe*

[a] Department of Chemical Sciences, University of Johannesburg, P.O. Box 524, Auckland Park 2006, Johannesburg, South Africa, Email: dipuopreciouskgabi@gmail.com

Keywords: bentonite, HDTMA, chromium, *E.coli*, TiO_2

Hexavalent chromium [Cr(VI)] and *Escherichia coli* (*E. coli*) are priority waterborne pollutants that threaten environmental and public health, especially in regions lacking advanced water treatment systems. While TiO_2-based photocatalysis is widely explored for Cr(VI) reduction, its application is limited by electron–hole recombination, dependence on external hole scavengers, and particle agglomeration [1]. In this work, we developed a novel titanium dioxide–silver/hexadecyltrimethylammonium-bentonite (TiO_2-Ag/HDTMA-Bt) composite with intrinsic hole-scavenging properties, designed to simultaneously adsorb and photoreduce Cr(VI) while inactivating *E. coli*.

The composite was synthesized by hydrolysis-derived TiO_2 nanoparticles integrated with Ag-modified, cationic surfactant–modified bentonite (**Figure 1**). Comprehensive characterization confirmed successful material fabrication and pollutant interactions. Batch experiments under ultraviolet light-emitting diode (UV-LED) irradiation demonstrated that the composite achieved 98% Cr(VI) removal at optimized conditions, outperforming Ag/HDTMA-Bt alone, while maintaining reusability for up to eight cycles. Spectra obtained from x-ray photoelectron spectroscopy revealed the co-existence of Cr(VI) and Cr(III), confirming coupled adsorption–reduction as the removal pathway. Furthermore, antibacterial studies showed complete *E. coli* disinfection at a minimum inhibitory concentration of 0.16 mg/mL, attributable to Ag incorporation.

This multifunctional composite offers a low-cost, environmentally friendly, and highly efficient strategy for addressing both chemical and microbial water contamination. Its synergistic adsorption–photocatalysis–disinfection performance highlights strong potential for sustainable water treatment applications.

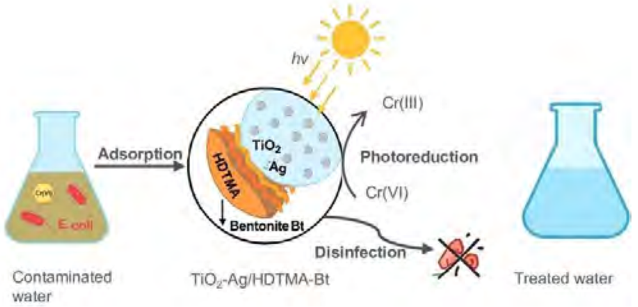

Figure 1: Schematic illustration of the TiO_2-Ag/HDTMA-bentonite composite showing the synergistic mechanisms of Cr(VI) adsorption–photoreduction and antibacterial disinfection of *E. coli* under UV irradiation.

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Quantum dot-based sensors: synthesis, characterization and application for the detection of organic pollutants in environmental samples.

Sifiso A. Nsibande *and Patricia Forbes*

[a] Department of Chemistry, Faculty of Natural and Agricultural Sciences, University of Pretoria, Lynnwood Road, Pretoria, 0002, South Africa. E-mail: sifiso.nsibande@up.ac.za

Keywords: quantum dot, sensor, organic pollutant, pesticide, polycyclic aromatic hydrocarbon

Environmental pollutants like pesticides and polycyclic aromatic hydrocarbons (PAHs) require continuous monitoring due to the potential harm they pose to the environment, aquatic life and human health. Thus, there is a need to develop robust, cost-effective, and sensitive analytical techniques and methods that can be used for the screening of these compounds at low concentrations. To this end, quantum dots (QDs) offer unique chemical and optical properties that can be exploited in the development of nanoprobes to detect these compounds [1]. This work, therefore, showcases the synthesis, characterization and application of two examples of quantum dot-based sensors for analytical screening of organic environmental pollutants. Firstly, CdSeTe/ZnS core/shell quantum dot sensor, which was functionalized using molecularly imprinted polymer (MIP), and used for the detection of the pesticide atrazine [2]. The CdSeTe/ZnS@MIP sensor showed good sensitivity and selectivity for atrazine, allowing it to detect through fluorescence quenching, with a detection limit of 0.80×10^{-7} mol L^{-1}. In the second example, we prepared a carbon quantum dot (CQD) probe for the detection of pyrene in aquatic systems [3]. In this probe, a fluorescence "switch off-and-on" sensing strategy was employed where ferric ions were used to "turn off" or quench the fluorescence signal of the CQDs. Then, upon interaction of the quenched CQDs with pyrene, the fluorescence could be switched back on linearly with increasing pyrene concentration. Thus, this allowed for the development of a sensing strategy for pyrene where the limit of detection was 0.242×10^{-6} mol L^{-1}. Finally, the two sensors could be used in real environmental water samples where satisfactory recoveries were achieved, which were 92 – 118% for CdSeTe/ZnS@MIP and 97 – 107% for CQDs. This work demonstrates the potential of quantum dot-based fluorescence sensors to be used as analytical tools for screening pollutants in aquatic systems.

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rGO–IIP Nanocomposite Sensor: Tackling Cadmium Pollution in Water

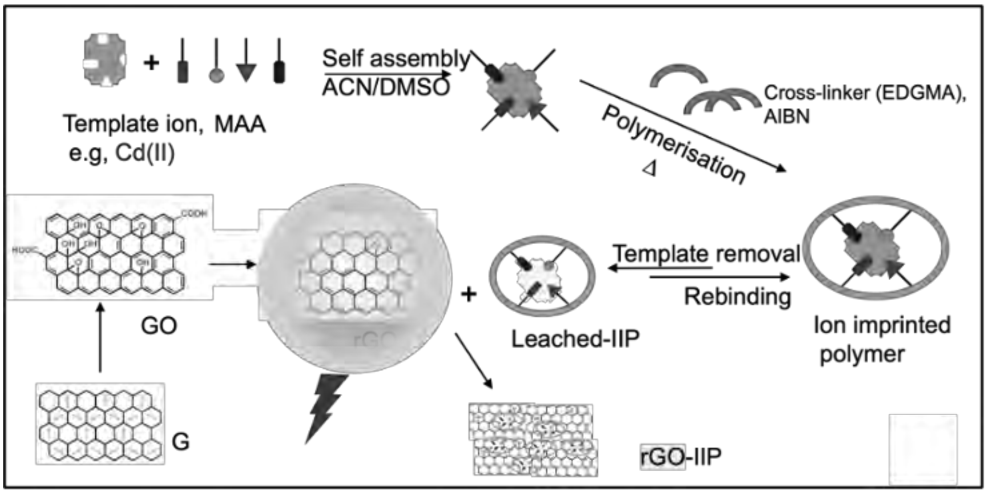
Sifelani Dube, Abayneh A. Ambushe and Messai A. Mamo

[a] Department of Chemical Sciences, University of Johannesburg, South Africa, E-mail: sifelanid@uj.ac.za.

Keywords: cadmium, chemiresistor, nanocomposite, graphene

Cadmium (Cd) contamination in water remains a critical environmental and public health challenge due to its high toxicity and persistence. Conventional analytical techniques, while accurate, are costly, laboratory-bound, and unsuitable for real-time field monitoring [1]. This work reports the development of a portable chemiresistive sensor integrating electrochemically reduced graphene oxide (rGO) with an ion-imprinted polymer (IIP) for detection of ultra-trace level Cd(II) in water. The optimized 1:3 IIP:rGO nanocomposite, drop-cast onto interdigitated gold electrodes, exhibited rapid response times (<60 s), excellent reproducibility (%RSD < 2.1%), and long-term stability (<10% drift over 90 days). The sensor demonstrated high selectivity against competing ions and achieved a low detection limit of 0.704 μgL^{-1}, below the WHO and SANS drinking water guideline (3 μgL^{-1}). Percentage recovery studies by spiking Cd(II) in borehole and river water confirmed the accuracy of the method and its applicability for environmental monitoring (95.9–103%) [2]. These findings highlight the potential of rGO–IIP chemiresistive sensors as cost-effective, scalable tools for on-site water quality assessment, advancing sustainable pollution management and public health protection.

Structure Block/Scheme.



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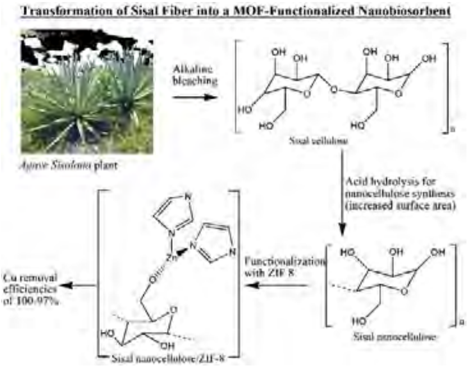
MOF-Functionalized Nanocellulose from *Agave Sisalana* Plant for Efficient Copper Removal from Treated Wastewater

Mothusi Molebatsi[ab], *Tlhabologo Moses Kabomo*[a], *Ngonye Keroletswe*[b] *and Samuel Chigome*[b]

[a]Department of Chemistry, University of Botswana, P/ Bag 0029, Gaborone, Botswana, 200600974@ub.ac.bw
[b]Natural Resources and Materials Division, *Botswana Institute of Technology Research and Innovation, P/Bag 0082, Gaborone, Botswana,* mmolebatsi@bitri.co.bw

Keywords: cellulose, heavy metals, metal organic framework, water treatment, sustainable remediation

Heavy metal contamination in water systems remains a significant environmental concern, especially in regions where industrial and pharmaceutical discharges are on the rise. In this study, cellulose was extracted from the *Agave Sisalana* plant and converted into nanocellulose, which was subsequently functionalized with a metal organic framework (MOF) called Zeolitic Imidazole Framework (ZIF-8) to develop a sustainable biosorbent for Copper ions (Cu^{2+}) removal from treated wastewater. Three materials (sisal cellulose, nanocellulose, and MOF-functionalized nanocellulose) were characterized using FTIR, SEM, elemental analysis, TGA, solid-state NMR, and XRD planned for further structural analysis. Batch adsorption experiments were done using 0.5 g batches of each sorbent, with 10 mL of Cu^{2+} solutions (2- 100 ppm). The mixtures were agitated at 200 rpm at room temperature and without any pH adjustment. Cellulose achieved removal efficiencies of 98- 90% while nanocellulose achieved 89-92% for Cu^{2+} solutions of 2 to 100 ppm. Although cellulose performed better at low concentrations, nanocellulose outperformed it at higher concentrations (e.g., 50ppm), attributed to its higher surface area. The SEM revealed nanocellulose fiber diameters in the range of 20–50 nm, a significant reduction from the 10–50 µm observed for cellulose. This justified the further modification of nanocellulose with MOFs to maximize performance across a wider concentration range. Therefore, MOF-functionalized nanocellulose exhibited the highest removal efficiency of 100-97% due to additional functional groups providing more binding sites for Cu^{2+}. Kinetic studies, equilibrium isotherms, and thermodynamic analyses are also underway to determine the rate-controlling mechanisms of adsorption and adsorption capacities. This study underscores the potential of using natural, biodegradable cellulose-based materials enhanced *via* MOF integration for efficient remediation of toxic metals (Cu and Pb) from treated wastewater. The findings contribute to the advancement of green, nanotechnology-driven approaches in water treatment, with potential scalability for industrial applications



Exploration of plant *Eucalyptus cinerea* essential oil as a green, affordable, and sustainable adsorbent for the removal of antibiotics from wastewater

Lelethu Kontile and Precious Mahlambi

[a] Department of Chemistry, University of KwaZulu-Natal, Scottsville, Pietermaritzburg, 3201, South Africa, E-mail: 218022087@stu.ukzn.ac.za

Keywords: White silver (*Eucalyptus cinerea)*, adsorption, kinetics, isotherms

Sulfonamides (SAs) are antibiotics for treating human and animal bacterial infections. The high consumption and improper disposal of these antibiotics have made them common in aquatic environments. Conventional wastewater treatment processes cannot completely eliminate SAs; thus, this work aims to explore for the first time the essential oil of white silver as a green, inexpensive, and sustainable adsorbent for removing SAs in wastewater. Before adsorption studies, Fourier Transform Infrared (FTIR) spectroscopy, Gas Chromatography Mass Spectrometry (GC/MS), and Transmission Electron Microscopy (TEM) were performed for the characterisation of the essential oils. FTIR allowed for identifying functional groups such as O-H, C=C, and C-H, which can bind to sulfonamide antibiotics. GC-MS identified 1,8-cineole as the dominant compound, whose chemical structure enables adsorption. TEM for white silver showed that the surface area had rod-like shapes, enhancing the adsorption capacity. Prime factors affecting adsorbent abilities were evaluated: initial concentration of analyte, pH, contact time and volume of adsorbent. The relative recoveries of selected antibiotics were 89% and 109% for white silver. Adsorption kinetics were found to obey the pseudo-second order. Adsorption isotherms fit the Temkin model. This study shows that essential oils of white silver can be successfully employed as inexpensive, eco-friendly and viable adsorbents for removing SAs from wastewater.

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Fluoride Removal from Water by the Application of Bone Char Prepared from Wild Animal and Bird Bones

Sello Moloi[a,b], *Jonathan Okonkwo*[a] *and Ray Jansen*[a]

[a] Department of Environmental, Water and Earth Sciences, Faculty of Science, Tshwane University of Technology, Nelson Mandela Road, Arcadia, Pretoria, 0001, South Africa. [b]National Research Foundation, Meiring Naude Road, Brummeria, Pretoria, 0002, South Africa, E-mail: sello.moloi@nrf.ac.za

Keywords: bone char; adsorbent; fluoride, water, defluoridation

Fluoride contamination in drinking water poses significant health risks, particularly fluorosis, prompting the need for effective removal methods [1]. This study explores the use of bone char, derived from various animal bones, as a cost-effective and environmentally friendly adsorbent for fluoride removal. Hydroxyapatite, a calcium phosphate mineral prevalent in bones, is central to this process, with charring enhancing its crystallization and surface area for better fluoride ion interaction. When calcium ions (Ca^{2+}) are leached from bone char, fluoride ions (F^-) in water can precipitate as insoluble calcium fluoride (CaF_2). The research involved seven types of bones from livestock, wild mammals, and birds, which were processed into different particle sizes for testing.

Key findings from batch experiments revealed that the finest particles (≤150 µm) achieved a fluoride removal capacity of 26.8% under unoptimized conditions. Adjusting the pH to 2 significantly improved fluoride removal to 89.7%, while a fluoride concentration of 10 mg/L yielded an 82.3% removal efficiency. The optimal contact time for maximum fluoride removal was identified as 90 min, achieving fluoride removal capacity of 93.0%. An optimal adsorbent dosage of 1 g effectively removed 98-100% of fluoride from low-concentration solutions. The study also evaluated the adsorption capacities of different bone types using Langmuir and Freundlich isotherm models. The average separation factor (R_L) of 0.5436 and the correlation coefficient values (R^2) of 0.9884 revealed the favourability of adsorption ($0 < R_L < 1$) and the suitability of Langmuir model to experimental data ($0 < R^2 \approx 1$). Freundlich model parameters implied favourable adsorption and high affinity for fluoride ions by raw bones ($(1/n) < 1$) and the results further indicated surface heterogeneity ($n < 1$) and therefore, the possibility of pores even before charring.

Notably, when charred bone samples were tested under optimal conditions, they demonstrated significant defluoridation in spiked borehole water samples, with red hartebeest bone achieving a remarkable 99.3% removal rate. Charred wild animal bones outperformed bird and livestock bones. When compared with raw bones, charred bones generally exhibited higher fluoride removal capacities. Using antibiotics in domestic and semi-wild animals to treat and control clinical diseases and to enhance animal growth can affect bone composition. This creates differences in the bones of wild, semi-wild, and production animals.

Overall, the findings confirm that both raw and charred wild animal and bird bones can serve as effective adsorbents for fluoride removal from water. The charring process enhances the material's surface area, facilitating better fluoride ion access. However, the study notes the importance of monitoring calcium and phosphate levels in treated water, as these are byproducts of hydroxyapatite dissolution.

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Adsorbents Derived from Invasive Weeds for Pollutant Control

Eric Danso-Boateng, Andrew Ross, Flora Chitalu and Yuchen Zhang*

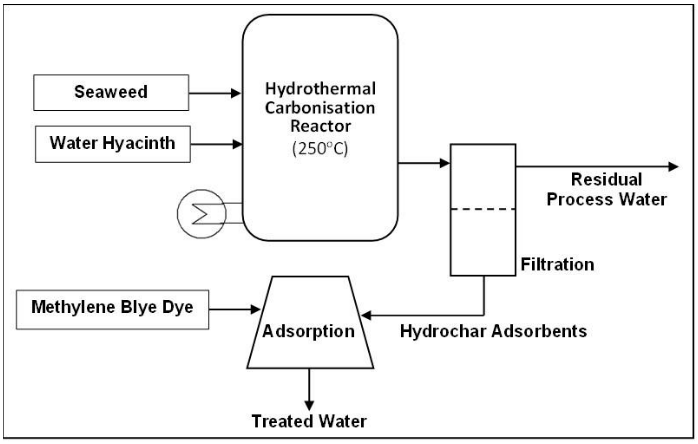
[a] School of Chemical and Process Engineering, University of Leeds, Leeds, LS2 9JT, UK. *E-mail: e.danso-boateng@leeds.ac.uk

Keywords: Adsorption, Hydrothermal carbonisation, Methylene Blue, Seaweed, Water hyacinth

Invasive weeds such as seaweed and water hyacinth are commonly available aquatic plants, which do not compete with land and food crops. Seaweed is available on most coastlines and can also be cultivated. However, a major concern is that if not removed in time, algae will decompose and emit odour, producing hydrogen sulphide, which is toxic and has adverse effects of coastal ecosystems. Water hyacinth, on the other hand, is a floating plant found in water bodies globally, and are dominant in regions where dye industries are prevalent. They form colonies that block sunlight from reaching water bodies and reduce oxygen level in the water. This affects water and various lifeforms in the ecosystem. It also results in increasing evapotranspiration of water bodies as well as creates favourable environment to produce mosquitoes and snails that cause diseases such as malaria and Bilharzia, respectively. Hence, utilisation of such evasive and abundant species as a useful resource would be a welcome solution. However, the composition of these invasive weeds differs from lignocellulosic biomass.

Therefore, considering the complexity and variability of their compositions, hydrothermal carbonisation (HTC) is utilised to covert seaweed and water hyacinth into “hydrochars” at processing temperatures up to 250ºC, to study their adsorption properties and their potential for adsorptive removal of methylene blue dye from aqueous solutions. The hydrochars were characterised using scanning electron microscope, proximate and ultimate analyses, Fourier-transform infrared spectrometer, and BET surface area.

The study found that HTC temperature influence adsorbents properties. BET surface area increased at higher HTC temperature with values up to12.78 m^2/g and 3.807 m^2/g for hydrochars derived from seaweed and water hyacinth respectively. Adsorption results showed that adsorbents derived from the invasive weeds are effective for the removal of >99% of cationic methylene blue dye from aqueous solutions, which is influenced by pH and initial concentrations of the solution and contact time.



Magnetic carbon nanosheets derived from PET plastic waste for the preconcentration and adsorptive removal of selected trace metals in water

Naom Momanyi, Lawrence M. Madikizela and Titus A.M Msagati, Tshimangadzo S. Munonde[*]

[a] Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Florida Science Campus, Roodepoort 1710, South Africa, E-mail*: munonts@unisa.ac.za

Keywords: Magnetic nanostructured carbon, plastic waste valorization, UAMSPE, trace metals, wood preservatives, environmental monitoring

The release of toxic trace metals such as arsenic (As), chromium (Cr), and copper (Cu), amongst others into drinking water sources from wood-preserving industries poses significant environmental and public health risks [1], [2]. This study reports the successful synthesis, characterization, and application of a novel magnetic nanostructured carbon adsorbent derived from plastic waste for the preconcentration of these trace metals in environmental water samples. Plastic waste was converted into carbon-rich nanomaterials via hydrothermal treatment and pyrolysis, followed by magnetization with Fe_3O_4 nanoparticles to yield a reusable magnetic nanocomposite [3], [4]. Comprehensive characterization was performed using SEM/EDX, HR-TEM/SAED, XRD, FTIR, Raman, BET, XPS, VSM, and zeta potential analyses, confirming the successful formation of porous, crystalline, and magnetically responsive carbon-based materials with abundant surface functionalities for metal adsorption. The synthesized nano adsorbent was integrated into an optimized ultrasound-assisted magnetic solid-phase extraction (UAMSPE) protocol for the extraction and adsorption of As, Cr, Cu and other trace metals from water. Under optimized conditions, the developed UAMSPE method exhibited high extraction efficiencies (>90%), low detection limits (0.05–0.3 µg/L), good reproducibility (RSD < 5%), and rapid extraction times (<10 min). Application to drinking water samples collected near wood-treatment facilities across South Africa confirmed elevated levels of these metals, underlining the urgent need for regular monitoring and advanced analytical interventions. This study not only demonstrates the feasibility of converting plastic waste into high-performance nanomaterials but also contributes to the advancement of sustainable analytical methodologies for environmental surveillance of trace metal pollutants associated with industrial activities.

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Gas Chromatography for Decision-Grade Evidence in Cannabis Labeling and Human Pesticide Exposure

Mufaro Mugari[a], *Aqiel Dalvie*[b], *Nohlanhla Khumalo*[c] *and Maya Makatini*[d]

[a] Department of Medicine, University of Cape Town, Observatory, Cape Town, 7381, South Africa, E-mail: mufaro.mugari@uct.ac.za . [a]Department of Medicine, University of Cape Town, Observatory, Cape Town, 7381, South Africa, E-mail: aqiel.dalvie@uct.ac.za . [a]Department of Medicine, University of Cape Town, Observatory, Cape Town, 7381, South Africa, E-mail: n.khumalo@uct.ac.za. [a]Department of Chemistry, University of Witwatersrand, Braamfontein, Johannesburg, 7381, South Africa, E-mail: maya.makatini@wits.ac.za .

Keywords: GC-MS/MS, cannabis products, pesticides biomarkers, urine, cannabinoids, children

Gas chromatography–mass spectrometry (GC–MS) underpins product safety assessment and the monitoring of human exposure to chemicals of concern. This work describes the development, validation, and application of robust GC–MS workflows for two public-health priorities. First, a quality-control method for cannabis oils targets residual solvents and terpene profiles. Hexane-diluted extracts are analysed by optimized split/splitless liquid injection; conditions (inlet temperature, split ratio, liner deactivation) are tuned against headspace operation to suppress thermal/inlet artefacts in terpene-rich matrices and reduce false positives for residual solvents.

Second, a biomonitoring method quantifies selected pesticide and plasticizer metabolites in human biological matrices, using matrix-appropriate QuEChERS and solid-phase extraction (SPE) for efficient clean-up. Both workflows are validated for fitness-for-purpose, demonstrating linearity, repeatability, recovery, and practical limits of detection and quantitation; quantitative results are reported with associated measurement uncertainty to support interpretation near decision limits. Together, these methods provide defensible and transferable protocols that laboratories can implement readily, delivering reliable data to inform regulatory and clinical decision-making.

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Phytochemical investigation and biopharmaceutical profiling of secondary metabolites from *Pappea capensis* for anticancer properties

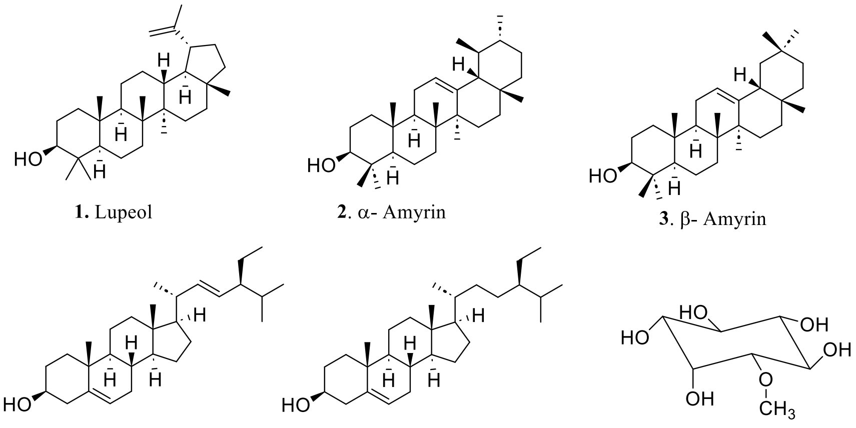
Lethabo Masemola[a], *Clemence Tarirai*[b], *Xavier Siwe Noundou*[c] *and Jacqueline Tembu*[a]

[a] Department of Chemistry, Tshwane University of Technology, Pretoria, South Africa, E-mail: masemolal96@gmail.com
[b]Department of Pharmaceutical Sciences, Tshwane University of Technology, Pretoria, South Africa. [c]Department of Pharmaceutical Sciences, Sefako Makgatho Health Sciences University, Pretoria, South Africa.

Keywords: *Pappea Capensis*, Triterpenoids, Steroids

Cancer is a major global health concern for several reasons such as increasing incidence and lack of effective treatment. Since the discovery of anticancer agent i.e. taxol, isolated from *Taxus brevifolia*, the search for anticancer metabolites from medicinal plants has increased drastically [1]. *Pappea Capensis*, the only species of the genus *Pappea* is a tree commonly known as Jacket plum and belongs to the Sapindaceae family. *P. capensis* extracts have been reported to possess anticancer activity. [2]. Thus, this study aimed at extracting and identifying bioactive secondary metabolites from *Pappea capensis* for anticancer properties and their encapsulation into nanostructured drug delivery systems.

Dried and grounded aerial parts (4.33 kg) of *P. capensis* were sequentially extracted with hexane, dichloromethane, ethyl acetate and methanol. Dichloromethane, Ethyl acetate and methanol extracts were fractionated and purified using column chromatography (CC) and thin layer chromatography (TLC). The characterization of isolated compounds using nuclear magnetic resonance (NMR) and infrared spectroscopy resulted in identification of three pentacyclic triterpenes: Lupeol (**1**), mixture of α-Amyrin (**2**) and β-Amyrin (**3**), steroids: stigmasterol **(4)**, β-sitosterol (**5**), and a cyclitol; Bornesitol (**6**) as shown in Figure 1. The isolated compounds were encapsulated into chitosan and liposome nanoparticles. Encapsulation efficiency, *in vitro* drug release and permeability were determined. Crude extracts and isolated compounds will be evaluated for *in vitro* anticancer properties.



1. Lupeol **2**. α- Amyrin **3**. β- Amyrin

4. Stigmasterol **5**. β-Sitosterol **6**. Bornesitol

Figure 1: Compounds isolated from *P. capensis*

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Photodegradation Kinetics of Amoxicillin, Carbamazepine and Diclofenac Under Simulated Solar Light: Fluorescence EEMs Deconvolution Insights

Ntsieni Romani Molaudzi, *Mathapelo Pearl Seopela and Abayneh Ataro Ambushe*

[a] Department of Chemical Sciences, University of Johannesburg, P.O. Box 524, Johannesburg 2006, South Africa, E-mail: ntsieni.molaudzi6@gmail.com

Keywords: photodegradation, fluorescence EEM, PARAFAC analysis

Pharmaceutical contamination in aquatic environments presents a significant risk to water quality, ecosystem health, and public safety. Pharmaceuticals persist in surface waters as a result of their widespread consumption, incomplete metabolism, and ineffective removal during conventional wastewater treatment processes [1]. This study explored the photodegradation behaviour of three widely used pharmaceuticals: amoxicillin (AMO), carbamazepine (CAR), and diclofenac (DIC), using a custom-designed photoirradiation system that simulates solar conditions. Each compound was investigated at a concentration of 1.00 mg/L, both in the absence and presence of 1.00 mg/L of Suwannee River natural organic matter (SRNOM), to assess the influence of natural components on degradation processes. Throughout the 8.1-hour exposure period, changes in the aqueous systems were monitored using simultaneous fluorescence excitation-emission matrix (EEM) spectroscopy and UV-Vis absorbance at 18-minute intervals. To deconvolute complex fluorescence data, parallel factor analysis (PARAFAC) was employed. The PARAFAC analysis enabled real-time monitoring of both parent compounds and their photoproducts by decomposing complex EEM datasets [2].

The results demonstrated distinct degradation behaviours across the three compounds. Amoxicillin degraded more rapidly than diclofenac, while carbamazepine remained relatively persistent. Although carbamazepine is not inherently fluorescent, several of its transformation products were detected through their fluorescence signatures. The presence of natural organic matter (NOM) had a variable effect on the photodegradation of the selected pharmaceuticals. The NOM inhibited the degradation of AMO and the fluorescent photoproducts of CAR, while accelerating the breakdown of DIC. These findings suggest that the excited states of NOM can significantly mediate photodegradation pathways. The detection of multiple fluorescent photoproducts, many with unknown toxicological profiles, underscores the potential environmental risks posed by pharmaceutical transformation in surface waters. This study highlights the value of combining spectroscopic techniques with PARAFAC analysis to examine degradation processes in complex water matrices. Such methods provide a powerful framework for understanding contaminant behaviour and informing future water quality monitoring and regulation efforts.

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Analysis of the structural and energetic properties of Carbofuran and its polymorphs

Oluwatoyin Akerele[a] *and Andreas Lemmerer*[a]

[a] Department of Chemistry, University of the Witwatersrand, Private Bag 3, PO Wits, 2050, South Africa, E-oluwatoyin.akerele@wits.ac.za

Keywords: carbofuran, non-covalent interactions, electronic properties.

The rise in mosquito variants developing resistance against insecticides has reduced the efficacy of the current insecticides and threatens the substantial progress made in controlling malaria disease in the 21st century [1, 2]. There is a need to develop new insecticides that will eliminate malaria vectors. The discovery of new polymorphs of the existing insecticide with insecticidal activity is more advantageous than developing new insecticides because it is less expensive and risky and does not involve new matter compositions [3, 4]. In addition, studies have shown the polymorphs of insecticides are more effective against insects than the commercially available ones [4-6]. In this study, we discover two polymorphs of carbofuran through the slow-evaporation crystallization method, and their structural-property relationships were analyzed. The geometry of the experimental structures was in excellent agreement with the calculated geometry of the molecules at the M06l-D3/def2-TZVP level of theory. The packing arrangement of the commercially available carbofuran (Form **II,** melting point is 141.87) is different from the novel polymorphs (Form **I** (melting point is) and Form **III** (melting point is 138.51)), as shown in Fig. 1.

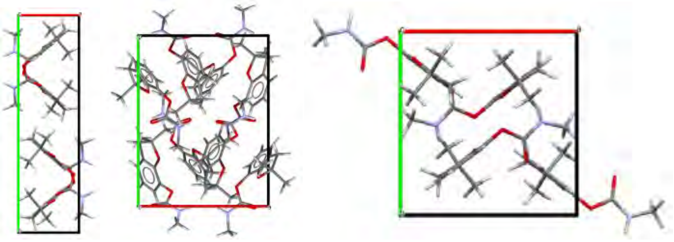
(a) (b) (c)

Figure 1: Crystal packing view along the *c*-axis of the crystal structure (a) new Form **I** (b) previously known Form **II** (c) new Form **III**

The theoretical investigation of energetic properties of the three forms reveals a decrease from Form **I** to Form **III**, which correlates with the result obtained from the differential scanning calorimetry (DSC) analysis: Form **I** (-31.76 kJmol^{-1}), Form **II** (-27.52 kJmol^{-1}), and Form **III** (-24.89 kJmol^{-1}). This suggests that the structures are chemically stable; however, the stability decreases from the new Form **I** to the existing Form **II** and then to the new Form **III**. The discovery of stable polymorphs means that a smaller amount of the compound will be used during application, which may reduce resistance since a large amount of insecticides is a major factor contributing to resistance development [7].

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A Tale of Two Polymorphic Pharmaceuticals: The Solid State Organic Chemistry of Persedon and Propylphenazone.

Andreas Lemmerer

[a] Jan Boeyens Structural Chemistry Laboratory, School of Chemistry, University of the Witwatersrand

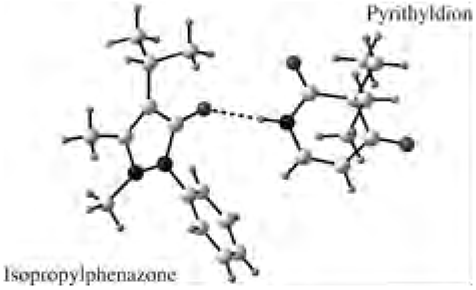
Keywords: structures, perspectives, reactions, selectivities

Kuhnert-Brandstätter and Burger investigated the polymorphs of Pyrithyldion, a sedative-hypnotic drug sold as Persedon®. Pyrithyldion exists as four polymorphs. The three crystalline polymorphs (and a plastic phase) can be obtained by careful manipulation of the crystals on the hot stage microscope. Form **II** is obtained from solution and **I** and **III** can be grown from the melt. The crystal structures of the three forms have not been determined previously and the focus of this contribution will be the description of their single crystal structures.

Propylphenazone is an analgesic derivative of phenazone and was studied by Müller and Beer. Three polymorphs have been identified, form **II** is the commercially available one and is the most stable. By cooling from the melt, mixtures of metastable forms **I** and **III** are obtained, together with form **II**. Form **I** and **III** convert back to form **II** after a few weeks. Solution experiments have failed to yield single crystal suitable for single-crystal X-ray diffraction. Hence, obtaining crystals and phase pure material of the individual polymorphs is difficult. However, the use of synchrotron powder diffraction on powder samples has helped to determine the crystal structure of at least two of the three forms.

The thermodynamic properties of the seven polymorphs and the phase relationships between the polymorphs of the two compounds have been determined by Differential Scanning Calorimetry.

Lastly, the co-crystal of these two pharmaceutical components - which was one of the first patented pharmaceutical co-crystals - is reported.



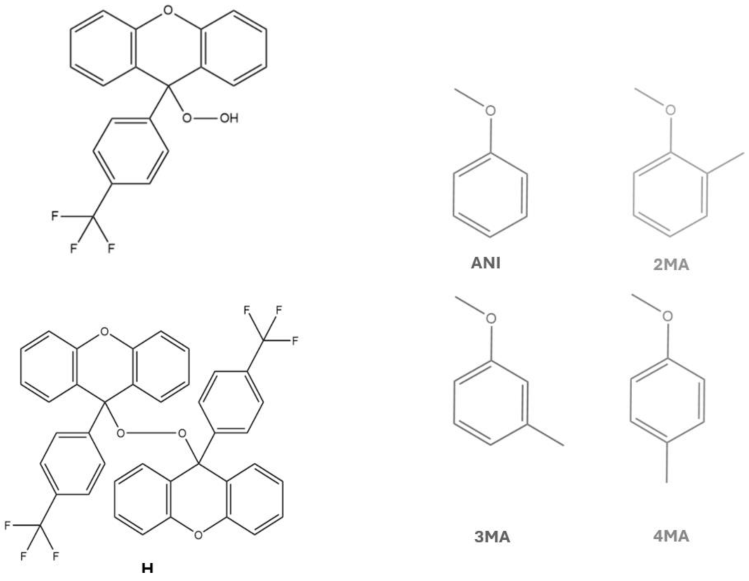
Peroxides as Host Compounds: An Investigation of the Host Ability and Selectivity of Di-(9-(p-trifluoromethylphenyl)xanthen-9-yl Peroxide in Mixed Anisole/Methylanisoles

Jarryd A. Vorgers, Benita Barton and Eric C. Hosten

[a] Department of Chemistry, PO Box 77000, Nelson Mandela University, Gqeberha (Port Elizabeth), 6031, South Africa.
E-mail: s219615039@mandela.ac.za

Keywords: Host-guest; Supramolecular; Anisole; Methylanisole; Separation; Peroxide

The present investigation focussed on the complexation behaviour of a peroxide, specifically di-(9-(*p*-trifluoromethylphenyl)xanthen-9-yl) peroxide (**H**), as a host compound for the potential guest species (anisole) ANI and 2-, 3- and 4-methylanisole (2MA, 3MA and 4MA) through crystallization experiments from each of these organic solvents. The results obtained demonstrate that **H** has the ability to form 1:1 host:guest inclusion complexes with each of ANI and 4MA, while no enclathration was observed when the guests were 2MA and 3MA. Furthermore, it was established from crystallization experiments in mixed guests that **H** possesses an overwhelming affinity for ANI followed by 4MA; equimolar mixed guest experiments showed the host selectivity to thus be in the order ANI > 4MA > 3MA > 2MA. Importantly, **H** was also shown to have the ability to separate 20:80 ANI:2MA and 60:40 4MA:2MA mixtures, in favour of ANI and 4MA, respectively (high selectivity coefficients, K, were calculated in these two instances). Single crystal X-ray diffraction (SCXRD) analyses indicated that 4MA engages in one (host)C–H···π(guest) and one (guest)C–H···π(host) interaction, while the overwhelming selectivity for ANI was attributed to the existence of two stabilizing (host)C–F···π(guest) bonds. Furthermore, thermoanalytical experiments demonstrated that the ANI-containing inclusion complex was significantly more stable than that with 4MA, explaining the host selectivity witnessed in the mixed guest experiments.



Scheme 1 Molecular structures of 9-hydroperoxy-9-(4-(trifluoromethyl) phenyl)-9H-xanthene, di-(9-(p-trifluoromethylphenyl) xanthen-9-yl peroxide (H) and the potential guest solvents ANI, 2MA, 3MA and 4MA.

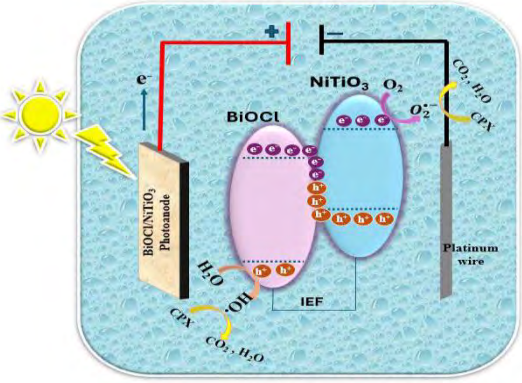
Integrated Z-scheme BiOCl/$NiTiO_3$ heterostructured photoanode and its photoelectrocatalytic application in ciprofloxacin degradation

Babatope O. Ojo[a], Nonhalangabezo Mabuba[a]

[a] Department of Chemical Science, University of Johannesburg, South Africa

Keywords: heterostructure photocatalyst, photoelectrocatalysis, water remediation

In this work, we explored the application of a novel BiOCl/$NiTiO_3$ heterostructured photoanode fabricated from the interfacial combination of BiOCl and $NiTiO_3$ semiconductors for the photoelectrocatalytic (PEC) degradation of ciprofloxacin in water. The choice of these semiconductors for heterostructured photoanode engineering originated from their unique structural and light absorption properties. Ciprofloxacin was equally targeted due to its frequent detection in various environmental waterbodies. Upon formation of BiOCl/$NiTiO_3$ heterostructured photoanode, a remarkable synergistic advantage and exceptional band alignment suitable for PEC application were obtained. These properties were confirmed by the impressively lower charge transfer resistance ($R_{ct} = 157\ \Omega$) and band gap energy (2.08 eV) possessed by BiOCl/$NiTiO_3$ heterostructured photoanode than the individual BiOCl and $NiTiO_3$ semiconductors. Moreover, these advantages agree with the exciting photocurrent density obtained for the heterostructured photoanode over individual photoanodes from various electrochemical and photoelectrochemical analyses. Furthermore, the deduced scheme of the BiOCl/$NiTiO_3$ heterostructured photoanode agrees with a Z-type behaviour, apparent from the spontaneous ease of electron migration from the conduction band of BiOCl (with a higher Fermi level) to the valence band of $NiTiO_3$ (with a lower Fermi level). Consequently, separated holes at the valence band of BiOCl and electrons at the conduction band of $NiTiO_3$ readily reacted with dissolved oxygen and water to form hydroxyl and superoxide radicals in the PEC system. This led to an impressive 94% removal efficiency after 120 min of applying the heterostructured photoanode for 5 mg L^{-1} ciprofloxacin degradation in water. Additionally, the heterostructured architecture displayed outstanding stability and reusability, positioning it as a promising advanced material for real-time applications.



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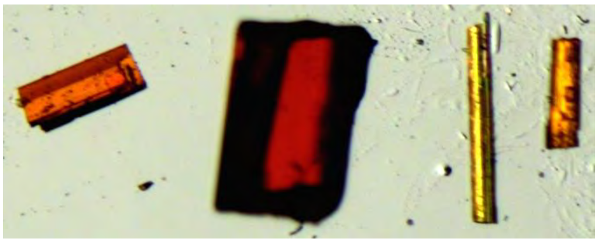
Polymorphism In Ternary Complexes

Atiyyah Salajee[a], *Rudolph Erasmus*[b], *Andreas Lemmerer*[a]

[a] Jan Boeyens Structural Chemistry Laboratory, Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, PO Wits, 2050, Johannesburg, South Africa.
[b]School of Physics, University of the Witwatersrand, Private Bag X3, Wits, 2050, Johannesburg, South Africa.

Keywords: crystal engineering, polymorphism, single crystal x-ray diffraction.

The design and synthesis of multi-component complexes, in particular cocrystals, has become an area of great interest in recent years, due to their potential of enhancing the physiochemical properties of the starting components. Multi-component complexes have the potential to crystallize in more than one form, known as polymorphism. In this work, crystal engineering techniques were exploited to synthesize ternary complexes of 1,3,5-trinitrobenzene (**tnb**), 9-anthracenecarboxylic acid **(9-aca**), and 3-hydroxypyridine (**3hp**). By varying the crystallization conditions such as the solvent, the temperature, evaporation rates, etc. polymorphs of these ternary complexes were envisaged. The analytical techniques: Single Crystal X-ray Diffraction (SCXRD), Powder X-ray Diffraction (PXRD), Hot Stage Microscopy (HSM), and Differential Scanning Calorimetry (DSC) were employed to characterize these ternary complexes and screen for polymorphs. In all complexes **9-aca** displays a charge transfer interaction with **tnb** and proton transfer to the pyridine. Two polymorphs of the ternary molecular salt cocrystal (3-hydroxypyridinium)·(9-anthracenecarboxylate)·(trinitrobenzene) were isolated. Form **I** crystallises as orange needles/rods, form **II** crystallises as red blocks, and forms **III** and **IV** both crystallise as orangey-yellow needles. Differential scanning calorimetry indicates that form **II** is the thermodynamically most stable form. Photoluminescence and UV-Vis studies showed that the polymorphs exhibit differing band gaps, correlating with their observed colours and electronic structures. These results emphasize the role of polymorphism in modulating the physical and chemical properties of multi-component molecular crystals.



Python-Based Quantum Chemistry Software in the Era of Quantum Computing: Educational Tools, Platforms, and Research Integration

Cyprian B. Moyo[a], *Karabo Bopape*[b], *Allen Gordon*[a], *Tendai O. Dembaremba*[a], *Adeniyi Ogunlaja*[a], *and Zenixole Tshentu*[a]

[a] Department of Chemistry, Nelson Mandela University-South Campus, Summerstrand, 6001, Gqeberha, South Africa, E-mail: cyprian.moyo@nithecs.ac.za. [b]RWTH Aachen University, Aachen, 52062, Germany.

Keywords: quantum chemistry, Python, PySCF, quantum computing, educational software, HPC integration,

The landscape of quantum chemistry education and research has undergone transformative changes in 2023-2025, driven by revolutionary developments in Python-based software packages, quantum computing platform accessibility, and hybrid classical-quantum algorithms. [1,2] Herein we present latest advances in educational quantum chemistry tools, focusing on PySCF's groundbreaking GPU acceleration achieving 50X speedup, [3,4] emerging quantum computing platforms from IBM, Microsoft, and Google offering unprecedented educational access, [5,6] and the integration of high-performance computing with quantum technologies. [7] The designation of 2025 as the International Year of Quantum Science and Technology has catalyzed global educational initiatives, while new interactive platforms like eChem and GPU4PySCF are democratizing access to advanced computational chemistry. [8] Research identifies over $49 billion in global investment driving quantum education initiatives, creating demand for 250,000 new quantum professionals by 2030. [9] This presentation analyzes recent developments in quantum algorithms for molecular computational sciences, examines the current state of quantum computing hardware capabilities, and evaluates new educational tools specifically designed for teaching quantum chemistry through computational methods. [5,7] The convergence of classical HPC and quantum computing presents unprecedented opportunities for chemistry education, with cloud-based platforms now providing students and researchers access to both classical supercomputing resources and quantum processing units (QPC's) through unified programming interfaces. [7,8]

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Molecular-wide chemical bond theory: Bridging the gap between atomistic chemistry and holistic physics

Jurgens H. de Lange[a]

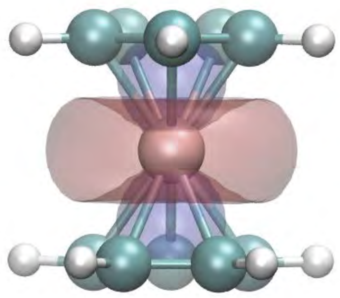
[a]Department of Chemistry, University of Pretoria, Hatfield 0002, South Africa, E-mail: jurgens.delange@up.ac.za

Keywords: theoretical chemistry, electron delocalization, chemical bond theory

Quantum mechanical modelling of complex chemical systems has never been more accessible due to increasing algorithmic efficiency, hardware capabilities and wide-spread availability of computational skills and training. Unbelievably, coupled-cluster and other multi-determinant electronic structure calculations can presently be performed, almost routinely, on proteins.[1] However, the interpretation of quantum chemical wavefunctions still remains a troublesome bottleneck to the wide-spread adoption of theory-first chemistry research. The prevalence of the molecular structure hypothesis (MST) – that molecules are comprised of atoms – are seemingly at odds with the molecular-wide nature of the wavefunction.[2] Within the Born-Oppenheimer approximation, this philosophical divide between reductionist chemistry and holistic physics boils down to the mathematical treatment and interpretation of electron delocalization.

We introduce here the Fragment, Atomic, Localized, Delocalized and Interatomic (FALDI)[3] density decomposition scheme as a theoretical instrument to bridge the language barrier between chemistry and physics. FALDI asserts that the electron density of an atom-in-a-molecule is simultaneously bounded and fuzzy. We present a mathematical framework for delocalized electron counting, population stockholding and visualization, thereby recovering the MST whilst including all of the information from the molecular wavefunction. We also show the relationship between molecular orbitals and molecular-wide atomistic descriptions. FALDI thereby is both a fundamental theory of electronic structure and an interpretative tool with high utility for human and artificial chemists alike.

We present aspects of the theory in a series of fun case-studies to highlight the molecular-wide nature of chemical interactions, including non-covalent interactions in DNA, molecular orbital interactions in ferrocene and CH---HC interactions in biphenyl.



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Impacts of aromatic bridges on electronic and nonlinear optical properties of Reichardt's types of zwitterionic molecules: a computational study

Divya Pant *and Sanyasi Sitha**

[a] Department of Chemical Sciences, University of Johannesburg, PO Box 524, Auckland Park, Johannesburg, South Africa 2006, Email: ssitha@uj.ac.za

Keywords: zwitterions, polarizability, hyperpolarizability, nonlinear optics

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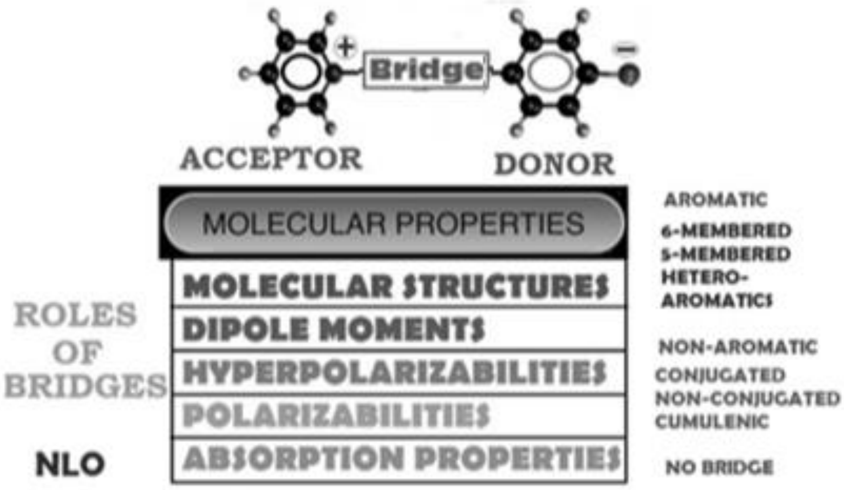
Based on many promising earlier studies [1-3], here we investigated a new series of donor–bridge–acceptor (D–π–A) types of zwitterionic molecules. Large hyperpolarizabilities or strong nonlinear optical (NLO) characteristics with possible optoelectronic applications, reported for such kinds of zwitterionic systems, by earlier studies clearly indicate the significance of the molecules studied here. The current study is focused on Reichardt-types of zwitterions, combined with a variety of aromatic and non-aromatic bridges. Our aim is to understand how different types of bridges influence the structural and electronic properties of D–π–A zwitterionic systems. The molecular design includes phenolate as the common electron donor (negatively charged) and pyridinium as the common electron acceptor (positively charged). A directly connected donor–acceptor molecule was used as a reference, and its properties were compared with those of bridged systems. Additionally, we compared our findings with a series of Brooker-types of zwitterionic molecules reported in the literature. Analysis of vertical excitations revealed that the nature of the bridging unit significantly affects the charge transfer characteristics and absorption maxima, which in turn strongly influence the linear and nonlinear optical responses of these molecules. All computations were performed using various quantum mechanical methods, including HF, B3LYP, CAM-B3LYP, and ωB97X-D, implemented through the Gaussian 09 software program.



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Catalytic Performance of Nanostructured Fe_x-$Mo_{0.1}$/TiO_2-Al_2O_3 Systems in Dibenzothiophene Hydrodesulfurization

Siphumelele Majodina[ab], *Jaco Olivier*[c], *Zenixole Tshentu*[a] *and* *Adeniyi S. Ogunlaja*[a]

[a] Department of Chemistry, Nelson Mandela University, Gqeberha, South Africa, [b]Sasol Technology (Pty) Ltd, Sasolburg, South Africa [c]Department of Physics and Centre for High Resolution (HRTEM), Nelson Mandela University, Gqeberha (Port Elizabeth), South Africa. E-mail: adeniyi.ogunlaja@mandela.ac.za

Keywords: Hydrodesulfurization (HDS), $Fe_xMo_{1.0}$-TA (TiO_2/γ-Al_2O_3 0.8), Dibenzothiophene (DBT)

Deep hydrodesulfurization (HDS) of fuel oils continues to attract research interest due to environmental-driven regulations which limit its sulfur content in fuel to 10–15 ppm [1]. Herein, we report the synthesis of new HDS catalyst, $Fe_xMo_{1.0}$-TA (TiO_2/γ-Al_2O_3 0.8) (x = 0, 0.5, 1.0, and 1.5) via the incipient impregnation method. The catalysts were characterized by means of UV-vis, FTIR, XRD, N_2-adsorption-desorption, H_2-TPR, XPS, NH_3-TPD, SEM, EDS, TGA-DSC, and HRTEM. The prepared Mo/Fe-based catalysts were tested for their catalytic HDS activity on dibenzothiophene (DBT). From the catalyst activity-structure correlation, the improved activity of $Fe_xMo_{1.0}$-TA 0.8 (x=1.0) was attributed to the formation of more active phases (MoS_2) Mo^{4+} species, as shown by XPS analysis [2, 3]. The hydrodesulfurization (HDS) activity followed the order: $Fe_{1.0}Mo_{1.0}$-TA 0.8 (91%) > $Fe_{1.5}Mo_{1.0}$-TA 0.8 (90%) > $Fe_{0.5}Mo_{1.0}$-TA 0.8 (84%) > $Mo_{1.0}$-TA 0.8 (66%), with all catalysts favouring the HYD pathway (Fig. 1). This improved HDS performance in Fe-promoted catalysts stems from three key factors: (1) higher reducibility and sulfidation degree, (2) the presence of Ti^{3+} (confirmed by XPS), and (3) Fe-induced charge transfer to Mo. These effects collectively weaken Mo-S/FeMo-S bonds, promote sulfur vacancy formation (creating more coordinatively unsaturated sites, CUS), and ultimately enhance both HDS and HYD activities.

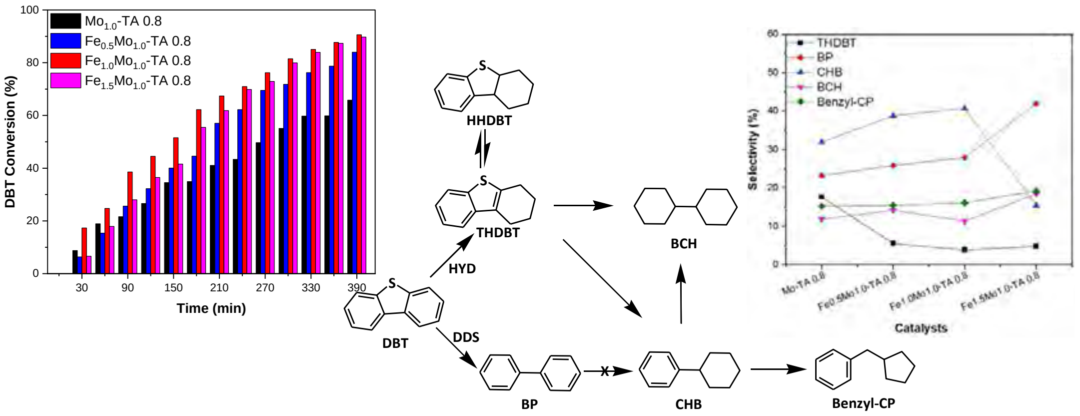

Fig 1 (a) Hydrodesulfurization conversion of DBT over prepared catalysts (T = 300 ºC, P = 3.5 MPa, m_{cat} = 2.0 g, heptane = 200 mL, and C_{DBT} = 550 ppm(S) using $Mo_{1.0}$-TA-0.8, $Fe_{0.5}Mo_{1.0}$-TA-0.8, $Fe_{1.0}Mo_{1.0}$-TA-0.8, and $Fe_{1.5}Mo_{1.0}$-TA-0.8 catalysts, (b) Proposed mechanism for catalytic HDS of DBT on Mo-based catalysts and (c) Product distribution of DBT HDS reaction.

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Sustainable Conversion of Waste Cooking Oil to Biodiesel Using Bifunctional Metal-supported MOF-Based Heterogeneous Catalysts

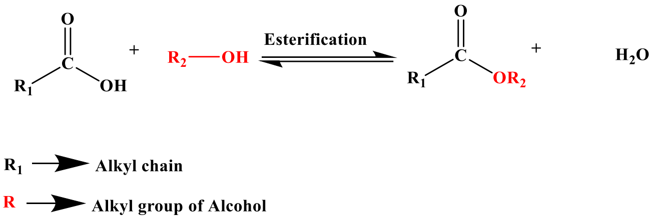
Abongile Gingqi[a], Azwihangwisi Mabunda[b], Shaine Raseale[c], Zondi Nate[a], Philani Mpungose[a]

[a]Department of Chemistry, Cape Peninsula University of Technology, Bellville Campus, Cape Town, 7535, mpungosep@cput.ac.za.[b]Department of Electrical Engineering, Cape Peninsula University of Technology, Cape Town, South Africa, mabudaa@cput.ac.za. [c]Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Rondebosch 7701, shaine.raseale@uct.ac.za

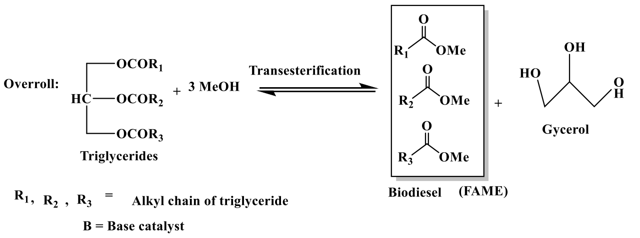
Keywords: Biodiesel, waste cooking oil (WCO), Metal organic framework (MOF), heterogeneous catalyst

The growing demand for renewable energy drives interest in biodiesel as a sustainable alternative to fossil fuels [1,2]. In this study, waste cooking oil (WCO), an abundant and low-cost feedstock, was converted into biodiesel through esterification and transesterification using a bifunctional heterogeneous catalyst, as shown in Schemes 1 and 2, respectively. The catalysts were synthesised by incorporating acidic (CuO) and basic (CaO) active components onto a UiO-66-based metal–organic framework (MOF). The three catalysts, Cu@UiO-66, Ca@UiO-66, and Cu-Ca@UiO-66, were successfully synthesised and fully characterised using XRD, BET surface area analysis, SEM, TEM, FTIR, XRF, NH_3-TPD, TGA, and particle size analyser.

These catalysts were then used to convert waste cooking oil to biodiesel. The formulation of these catalysts creates synergistic acid–base catalytic sites that enable efficient transesterification of triglycerides in a single step. Good to excellent yields were obtained, and the catalysts were efficiently recovered at the end of the reaction. Catalyst recovery and recyclability tests were also conducted, and all the catalysts were recycled three times without any significant loss of catalytic activity. Therefore, this study presents a green and economically viable approach to biodiesel production by converting waste into a valuable energy source through advanced catalyst engineering.



Scheme 1: An acid catalyst facilitates the esterification process [2].



Scheme 2: Base-catalysed reaction mechanism for the transesterification of triglycerides (TGs) [2].

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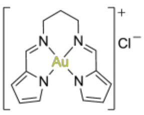
Biophysical studies of metal chelate binding by HSA: Towards an understanding of metallodrug transport

Sheldon Sookai[a], *and Orde Q. Munro*[a,b]

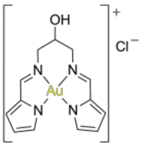
[a] Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, PO WITS 2050, Johannesburg, South Africa , E-mail: Sheldon.Sookai@wits.ac.za. [b] School of Chemistry University of Leeds, Woodhouse Lane, LS2 9JT, UK

Keywords: albumin, metallodrug, therapeutic, *in-silico*

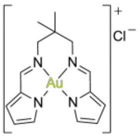
Human serum albumin (HSA) is the most abundant blood protein, transporting diverse endogenous and exogenous compounds, including many clinically used drugs. HSA significantly influences pharmacokinetics and pharmacodynamics, making the study of drug HSA interactions vital in drug development. This work describes the synthesis and characterisation of twelve Schiff base bis(pyrrolide-imine) metal complexes: five Au(III) [1,2], three Pt(II) [3], and one each of Ni(II) and Pd(II) [4]. Au(III) chelates, including a patented anti-cancer class, displayed moderate HSA binding (10^4–10^5 M^{-1}) and favoured Sudlow's site I. In NCI-60 screening, AuL1 and AuL3 showed cytotoxicity, with AuL1 acting as a topoisomerase II poison at low concentrations and a catalytic inhibitor at higher levels [1]. Two chiral Au(III) chelates exhibited taxol-like modes of action [3]. Pt(II) chelates, designed to explore theranostic potential, bound preferentially to Sudlow's site II [5], with affinities influenced by bis(imine) linker variations. Spectroscopic, docking, and ONIOM studies confirmed binding sites, and one complex acted as a UV-activated photosensitizer rather than a theranostic agent. The Ni(II) and Pd(II) chelates bound with affinities up to 10^6 M^{-1}, with the Pd(II) species showing unusually strong, enthalpy-driven binding attributed to London dispersion forces and a distinct binding mode. All complexes bound intact to HSA, suggesting their potential for HSA-mediated transport. These findings provide mechanistic insight into metallodrug protein interactions, highlighting how metal ion type, ligand architecture, and stereochemistry influence binding behaviour, stability, and biological activity offering guidance for the rational design of metallodrugs with improved delivery profiles.



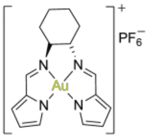
AuL1



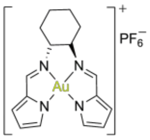
AuL2



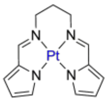
AuL3



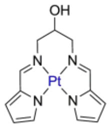
Au(1S, 2S-CyHex)



Au(1R, 2R-CyHex)



Pt(PrPyrr)



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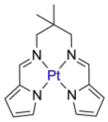

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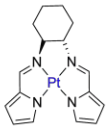

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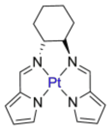

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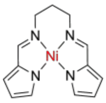
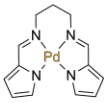


Ni(PrPyrr)



Pd(PrPyrr)

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Advancing Electrocatalysis: A Comprehensive Review of Metal (Cu, Co, Ni, etc) Nitrides, Sulphides, and Phosphides for Nitrate Reduction Reaction (NO_3RR) to Ammonia an alternative energy carrier

Wilson. M Seleka[a]; Nosipho Moloto[ab]; Izak Kotze[a*]; Postlet. M Shumbula[c*]; Edwin Makhado[c*]*

[a] Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Wits, 2050, South Africa,
[b] DSI/NRF Centre of Excellence in Strong Materials, University of the Witwatersrand, Braamfontein 2050, South Africa
[c] Department of Chemistry, University of Limpopo, Private Bag X1106 Sovenga, 0727, South Africa, Email 2225791@students@wits.ac.za

Keywords: Nitrate reduction reaction (NO_3RR) to ammonia; Ammonia yield; Faradaic efficiency (FE); Metal (i.e. Cu, Co, Ni, etc.)-based catalysts

The demand for a clean alternative energy carrier continues to be an ongoing challenge in the past and recently within the industries such as automobile, and portable power technologies. The utilisation of the traditional methods such as the one for producing carbon-based fuel energy possess negative drawback to the environment due to the emission of greenhouse gases which endangers the human health and the overall ecosystem [1-3]. However, the electrochemical nitrate reduction reaction to ammonia (NO_3RR) method is an emerging potential approach for sustainable ammonia production, offering an alternative to the energy-intensive through Haber-Bosch process [1-3]. This review explores metal (such as Cu, Co, Ni, etc.)-based catalysts attached to ligands such as nitrides, phosphides, and sulphides as a novel solution electrocatalysts materials for NO_3RR due to the superior properties they possess such as extensive turnable electronic structures, porous crystalline surface, and high conductivity. These novel materials are very selective, posses' high activity, and stability which makes them to be an ideal candidate for NO_3RR process.

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Nanocrystalline perovskites: the last man standing

Pierre Kalenga Mubiayi

[a] African Research Universities Association- Center of Excellence in Materials, Energy and Nanotechnology, School of Chemistry, University of Witwatersrand, Johannesburg, South Africa; Email: kalenga.mubiayi@wits.ac.za

Keywords: perovskites, preparation, green energy

Perovskite materials have played an important role in research and industries since the discovery of their properties from $BaTiO_3$. Technological challenges are being overcome by manipulating the properties of nanocrystalline perovskites through controlled syntheses and preparation of their composites such as those made of chalcogenides compounds. Stability is of the main factors hindering the use of perovskites in various activities. The stability of perovskites may be affected by environmental conditions, surface atomic structure, decomposition energy, etc. the interaction between atoms, the crystallinity and defects may be controlled to address the stability issues. Improving the performance of existing or new devices is the main aim set by scientists when studying nanoparticles. Inorganic perovskite nanocrystals were prepared via classical colloidal method and microwave assisted method. Various parameters of synthesis including the time, temperature, precursor concentration, coordinating solvent and capping agent were investigated. Their properties were studied and optimized for effective application in photovoltaic devices. Photocatalytic performance was evaluated from perovskite and their composites. Furthermore, several types of solar cell devices as well as perovskite cells were prepared from thin films of synthesized nanocrystals and evidence of photovoltaic activity was shown. The performance of fabricated devices was influenced by the structure of deposited thin films, especially the absorbing layer made of synthesized nanocrystals.

Design and synthesis of 8-quinoline-1,3,4-oxadiazole-thio-acetamide and ethanone derivatives as potential anti-HIV agents

Chakes Mashaba[a], *Matshawandile Tukulula*[a] *and Mabuatsela V Maphoru*[b]

[a] School of Chemistry and Physics, University of KwaZulu Natal, Westville Campus, Durban 4000, South Africa
[b]Department of Chemistry, Tshwane University Technology, Pretoria 0001, South Africa.

Keywords: 4-hycroxyquinoline, oxadiazole, hybridization.

Human Immunodeficiency Virus (HIV) remains one of the world's most challenging infectious diseases, despite decades of research and progress in treatment. Over 38 million people are currently living with the virus, and close to a million lives are lost each year due to AIDS-related complications [1]. One of the major challenges in managing HIV is its ability to mutate rapidly, leading to the emergence of drug-resistant strains. This growing resistance limits the effectiveness of existing therapies and highlights the urgent need for new and more potent compounds that act through different mechanisms. Developing innovative antiretroviral agents is essential to stay ahead of drug-resistance and to ensure better long-term outcomes for patients worldwide [2].

To this end, a small library of 8-quinoline-1,3,4-oxadiazole-thio-acetamide and ethanone derivatives were designed, synthesised and tested for their potential anti-HIV activities (Figure 1A and B). Synthesis involved a five-step synthetic protocol that resulted in compounds in yields ranging from 50-90%. Their structures were confirmed by 1D- and 2D-NMR, FTIR, and their masses validated by high-resolution mass spectrometry (HRMS). Few of these compounds showed promising IC_{50} activities against the HIV-1 sub-type B virus and appreciable cytotoxicity on TZM-bl cell lines.

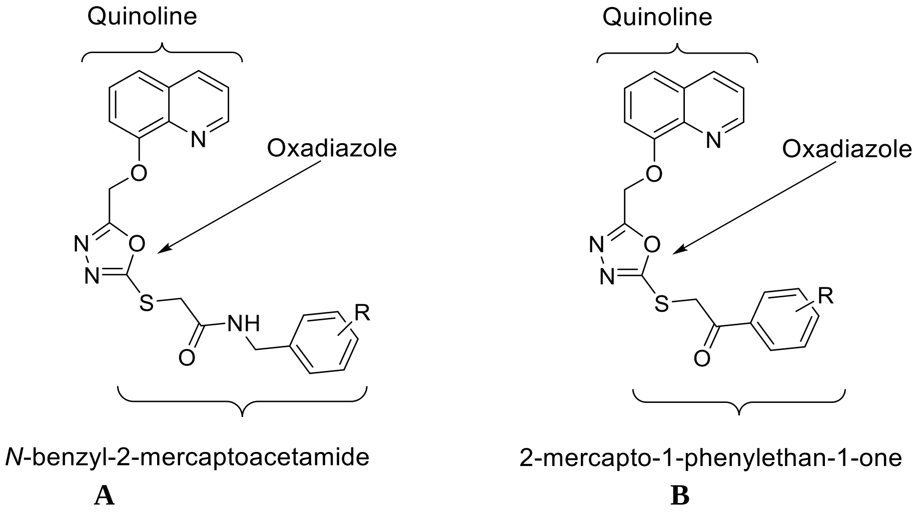

Figure 1: 8-Quinoline-1,3,4-oxadiazole-thio-acetamides and ethenone target compounds

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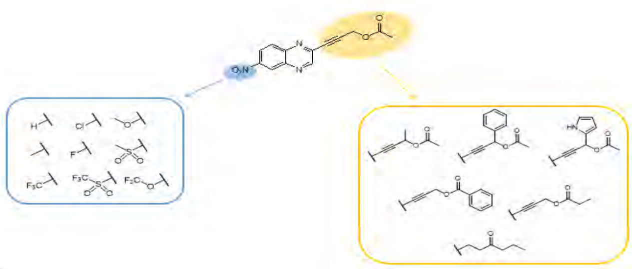
Synthesis and Biological Evaluation of Quinoxaline Derivatives as Potential Anti-Tuberculosis Agents

Blesant Kerryn Maluleke[a], *Winston Nxumalo*[a]

[a] University of Limpopo Private bag X1106 Sovenga 0727, E-mail: makerbkerryn@gmail.com; winston.nxumalo@ul.ac.za

Keywords: Quinoxaline, Mycobacterium tuberculosis, a minimum inhibitory concentration cytotoxicity, solubility

Quinoxaline derivatives have garnered significant interest in medicinal chemistry due to their wide range of pharmacological activities, including antitumor, anti-inflammatory, antimicrobial, and antiviral effects[1-3]. This study focuses on the synthesis of quinoxaline derivatives to evaluate their potential activity against tuberculosis (TB). The motivation for this research stems from our previous work on 3-(6-nitroquinoxalin-2-yl) prop-2-ynyl acetate, which exhibited promising anti-TB activity with a minimum inhibitory concentration (MIC) of 1.8 µM, a cytotoxicity IC50 of 13.5 µM, and a solubility of 195 µM [4]. The primary objective is to develop more effective anti-TB agents by synthesizing and evaluating a range of quinoxaline derivatives, thereby enabling structure-activity relationship (SAR) analyses to identify compounds with enhanced efficacy. The newly synthesized compounds were evaluated against Mycobacterium tuberculosis using the microplate alamar blue assay (MABA) to determine their MIC values. The MIC values of the synthesized compounds were determined, and their anti-mycobacterial activity were compared with standard drugs in use for TB treatment. Additionally, cytotoxicity and solubility studies were conducted on these compounds. The results indicated the synthesized quinoxaline derivatives demonstrated promising anti-tuberculosis activity, with certain structural modifications, such as the retaining of a nitro group at the 6-position enhancing their biological efficacy. While many compounds exhibited activity against Mycobacterium tuberculosis, their toxicity remains a concern that warrants further optimization. The findings suggest that specific functional groups, like alcohols, contribute to improved solubility, whereas reduction of alkyne groups tends to decrease activity but enhance solubility. Overall, these results provide valuable insights for the future design and development of more effective and safer anti-TB agents within the quinoxaline framework.



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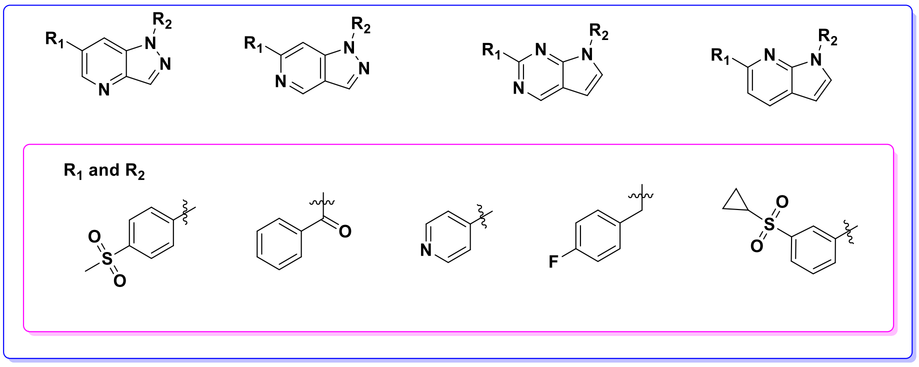
Design and synthesis of pyrazolopyrimidine, pyrazolopyridine pyrrolopyridine, and pyrrolopyrimidine derivatives as potential anti-malaria agents

Mabatamela LF[a], Nxumalo W[a]

[a] University of Limpopo, department of Chemistry, Private Bag x1106, Sovenga, 0727, Polokwane, South Africa, E-mail address: lebogangmabatamela0@gmail.com

Keywords: pyrazolopyridine, pyrrolopyridine, pyrrolopyrimidine pyrazolopyrimidine, NF54 strain.

Malaria is a disease that is caused by various *Plasmodium* species, with *Plasmodium falciparum* and *vivax* being the most prevalent. The disease is usually mostly severe in pregnant women and children under the age of five. The 2020 World Malaria Report from WHO estimated 241 million new malaria cases and 627000 malaria deaths globally. Emergence of resistance towards previously effective anti-malarial drugs, has resulted in an urgent need for the development of new drugs with new modes of action [1]. N-heterocycles systems have attracted considerable interest because they appear in many biologically active compounds and continue to serve as scaffolds for compounds displaying remarkable biological activities and are employed in a variety of pharmaceutical applications. Pyrazolopyrimidine, pyrazolopyridine, pyrrolopyridine, and pyrrolopyrimidine are all composed of N-heterocycles. These compounds have demonstrated anticancer, antibacterial, antiviral, anti-inflammatory, antifungal, and antihyperglycemic activities. In our previous studies, a series of imidazopyrimidine and pyrazolopymidine derivatives were successfully synthesised and tested for antimalarial activities and they showed good activities ranging from 0.009 to 6.0 μM [2]. This motivated us to explore these kinds of compounds even further, therefore we report on the synthesis of pyrazolopyrimidine, pyrazolopyridine, pyrrolopyridine, and pyrrolopyrimidine and their antimalarial activities.



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Power Compensation
Heat Flux
MMS 1
MultiSTAR

From Undergraduate Organic Chemistry to Functionalized Heterocycles

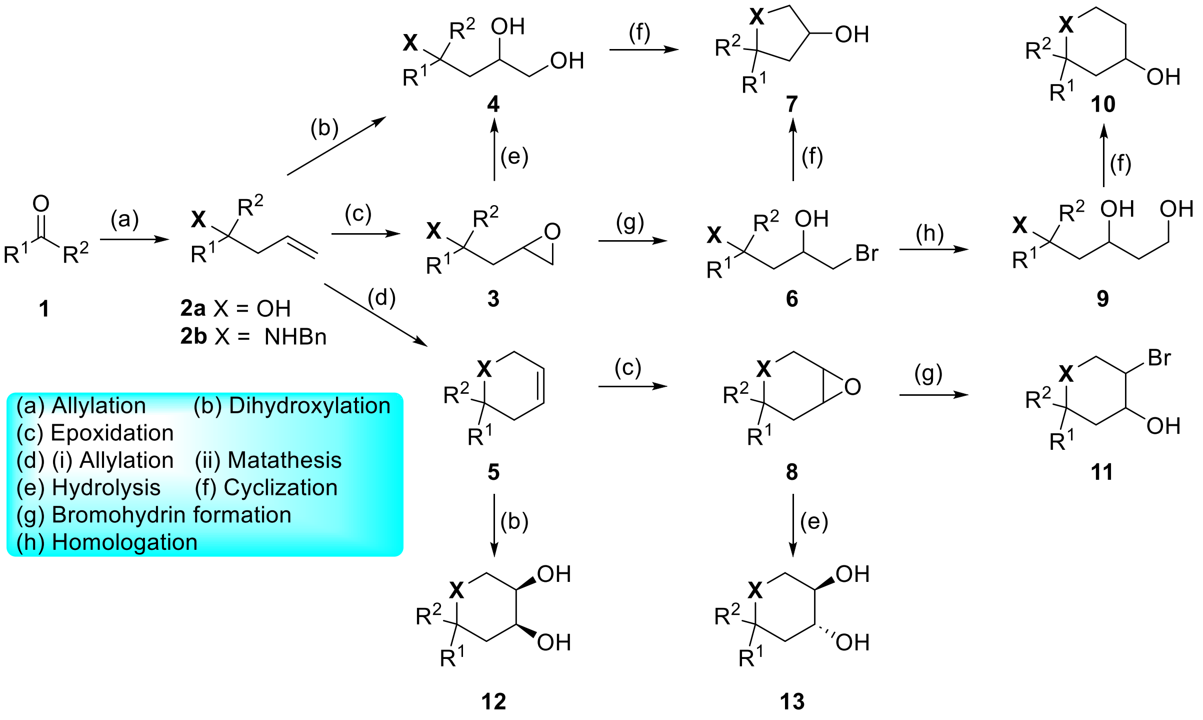
Nkwane Thobejane, Matumelo Ndlovu, Goitsemodimo Rakodi and Comfort Nkambule

[a] Department of Chemistry, Tshwane University of Technology, PB X680, Pretoria, 0001, South Africa
E-mail: Nkambulecm@tut.ac.za

Keywords: Heterocycles, Pyrrolidines, Tetrahydrofurans, Piperidines, Tetrahydropyrans

The practice of synthetic organic chemistry can be very expensive due to the reagents needed for very elegant syntheses published in high impact journals. This can be a daunting and discouraging challenge for organic synthesis researchers based in lower-income countries or universities. However, most undergraduate courses in organic chemistry are full of classical functional group transformation reactions using relatively inexpensive reagents.

Over the last 20 years the synthesis group at the Tshwane University of Technology (TUT) has pursued this "back to the roots" approach for the synthesis of chiral, functionalized heterocycles, summarized in Scheme 1.



Scheme 1 Simple organic chemistry applied for the synthesis of functionalized heterocycles

The presentation will highlight how standard "classroom" synthetic organic reactions were used for the synthesis of complex target small molecule heterocycles [1].

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Systems thinking for sustainability in chemistry education using green chemistry metrics and life cycle inventories of aspirin synthesis

Cathrine Chimude, Lynne Pilcher, Dorine Dikobe

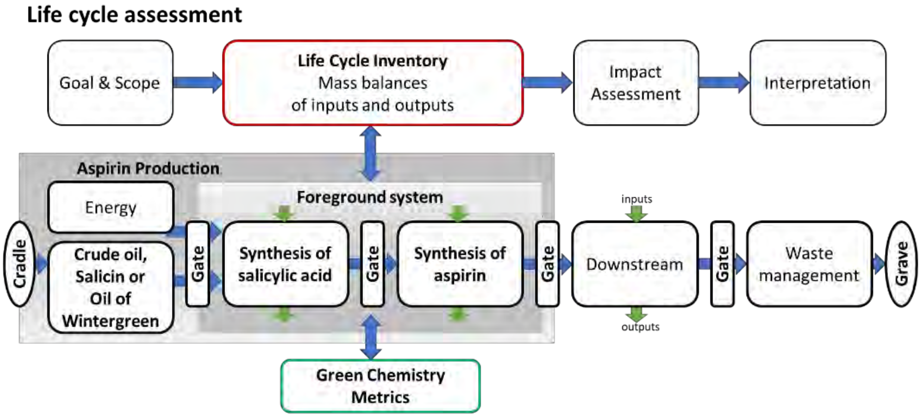
[a] Department of Chemistry, University of Pretoria, Pretoria, 0002, South Africa, E-mail: lynne.pilcher@up.ac.za

Keywords: systems thinking, first-year engineering, general chemistry

Systems Thinking is essential for addressing global sustainability challenges; however, opportunities to develop this skill set are not routinely included in chemistry curricula. It has been recognised as a key competency that should be intentionally cultivated in Education for Sustainable Development [1]. Students, particularly those who are not majoring in chemistry, tend to be more motivated to learn when they see the relevance of the subject to modern society [2]. Therefore, to introduce first-year chemistry students in engineering programs to concepts such as green chemistry, systems thinking, and sustainability in industry, we designed an activity centred around evaluating life cycle inventories for the production of aspirin using phenol, salicin, or oil of wintergreen.

To determine the effectiveness of the approach, we investigated the artefacts produced by students before, during, and after the group activity to find evidence of their engagement with Systems Thinking skills and their sense of responsibility towards achieving sustainability. Participant data were collected from 130 individual pre-practical exercises, 85 paired pre- and post-practical quizzes, and 20 group worksheets. We used deductive thematic coding and rubrics based on the Systems Thinking Hierarchical (STH) model [3] to analyse the data.

Our findings indicated that participants initially adopted a superficial approach to sustainability during the pre-practical phase, but their responses became more comprehensive in the post-practical phase. A paired T-test showed significant improvement in participants' systems thinking scores from pre- to post-practical quizzes. The deductive analysis using the STH model also revealed an enhancement in the quality of responses in the post-practical quizzes and group worksheets, indicating a transition from simplistic reasoning to holistic thinking. Furthermore, the analysis highlighted a positive shift in participants' attitudes toward collective responsibility for sustainability issues after the intervention. These results demonstrate that engaging with green chemistry metrics and life cycle inventories can effectively foster the development of Systems Thinking skills necessary for addressing sustainability challenges.



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Beyond the Curve: Unpacking Molar Absorptivity in HPLC

Shaeen Chetty[a], *Su-Ané Greyling*[a], *Letitia Pillay*[a]

[a] School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa. Email: shaeen.chetty1@wits.ac.za

Keywords: HPLC, organic acids, molar absorptivity, LoD, LoQ

In South African university analytical chemistry, third-year students typically learn about High-Performance Liquid Chromatography (HPLC) and its quantitative uses, such as calibration curves, limits of detection (LoD), and limits of quantification (LoQ). However, the fundamental concept of molar absorptivity (ε) is often not thoroughly explored in practical HPLC labs because it's challenging to design experiments that effectively demonstrate it. By demonstrating the interconnectedness of chromatography and spectroscopy, the knowledge of these techniques is reinforced.

We designed a new lab experiment to help students understand molar absorptivity and its role in analytical chemistry. Using common leaf samples, students were tasked with quantifying the organic acids they contained. This allowed them to practice basic sample preparation and learn about the factors involved in HPLC quantification. The main goal of the experiment was for students to directly observe how the molar absorptivity of different compounds visually impacts their ability to be quantified.

This experiment uses a constructivist teaching method, connecting students' prior knowledge of spectroscopy (like conjugation) from their second year directly to the practical applications of instrumental methods in their third year. For several years, this lab has successfully improved students' understanding of key HPLC quantification parameters, such as sample preparation, LoD, LoQ, and molar absorptivity. Students have also learned to recognize the impact of impurities on their results. This experiment has been met with positive student feedback, who reported increased interest and improved practical skills, including Excel proficiency. The approach also helps students develop a strong scientific methodology that applies to various fields of chemistry, from undergraduate to Honours-level studies. This teaching model effectively reinforces fundamental analytical concepts while showcasing their real-world applications in research and industry.

This presentation explains how a newly developed laboratory experiment, built on modern teaching practices, closes this gap. It helps students connect different analytical principles for a more comprehensive understanding.

Innovative teaching strategies for sustainable chemical education

Winifred Ifeoma Esiefa and Helen Drummond

[a] Department of Chemistry, North-West University, Mahikeng. South Africa. Email: winifeoma@gmail.com. Helen.Drummond@nwu.ac.za

Keywords: zwitterions, polarizability, hyperpolarizability, nonlinear optics

Achieving sustained development globally requires that United Nations SDGs 6, 7, 9, 13, 14 and 15 be routed through effective implementation of SDG 4. Knowledge about climate change, industrialization and the environment are crucial and these fundamental ideologies are tied together in chemical education. Chemical education equips learners with knowledge and abilities they need to accomplish global growth. Achieving SDG 4 requires activity-oriented, and learner centered strategies in teaching, which maximize self-development and fulfilment.

This study aims to examine innovative teaching strategies for sustainable chemical education. The innovative instructional strategy that is of interest in this study was the think-pair-share instructional strategy. The methodology utilized in this study was the quasi-experimental design of pretest post-test. The population of the study consists of 1,231 senior secondary school students, from which 173 samples were drawn using criterion-based random sampling. The instrument used for data collection was chemistry achievement test (CAT) on solubility, hydrocarbons, metals and their compounds. The data collected were analysed using SPSS V23. The mean achievement score of 75.57 was obtained with a standard deviation of 13.76 using think-pair-share strategy while 63.40 and 14.91 were obtained using the conventional teaching method.

The research revealed that students taught chemistry using the think-pair-share strategy achieved higher overall performance compared to those taught using conventional methods. The strategy enhanced their understanding through critical thinking, participation and confidence which means that the strategy was engaging. It is recommended that using the think-pair-share strategy in teaching and learning chemistry will foster a positive impact in chemical education and enhance global development.

Understanding the long-term development of high school teachers' insights into their PCK of chemical bonding

Marissa Rollnick[a], *Rene Toerien*[b] *and Annemarie Hattingh*[c]

[a] Wits school of Education, P.O. Wits 2050, South Africa, E-mail: marissa.rollnick@wits.ac.za [b]*Wynberg Boys' High School*, Cape Town, 7800 South Africa, E-mail: rene.toerien@gmail.com [c]School of Education, University of Cape Town, Rondebosch, 7701 Cape Town, South Africa.

Keywords: Pedagogical Content Knowledge, Chemical Bonding

Chemical bonding is a central concept in chemistry, but it is difficult to teach. The aim of this paper is to understand teachers' perception of a well-known representation of how/why atoms bond using two data sets collected 10 years apart. Part 1 of the study measured teachers' content and pedagogical content knowledge of chemical bonding using a validated diagnostic instrument, followed by interviews to determine the factors that influenced the teachers' perceptions of their Topic Specific Pedagogical Content Knowledge (TSPCK) for teaching chemical bonding. Part 2 of the study interviewed a sample of the teachers to detect development in their thinking a decade later. The first part of the study was framed in terms of older PCK models which have been superseded by new models and the effect of lifechanging events, especially COVID-19 and consequential technological changes that have changed teaching and learning, and hence teachers' understanding of how students learn basic concepts. This study addresses the question: What are teachers' reflections on the efficacy of a specific representation as a tool to assist learners' understanding of chemical bonding? The framework used was the Revised Consensus Model for PCK [2]. Five practising teachers consented to a second set of interviews which focused on a well-known representation, considered central to understanding chemical bonding. The teachers were asked to reflect on its efficacy for helping students understand chemical bonding (figure 1).

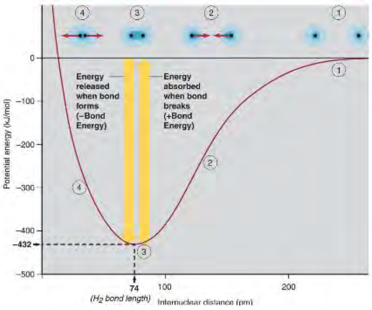

Figure 4: Why atoms Bond [1]

Only one of the teachers had a teaching qualification and none had a full chemistry major. The 2015 interviews were conducted in person, while the 2025 interviews were conducted online. Interviews were recorded, transcribed and analysed using commercial software. There were remarkable commonalities in the teachers' responses to the question about the representation. Four teachers said they used the diagram in teaching. Four of the five teachers considered the representation to have "too much going on" or having a "high cognitive load". Three teachers considered the idea of negative energy too challenging for learners. There was strong consensus on the difficulties in teaching the representation even though all considered it important

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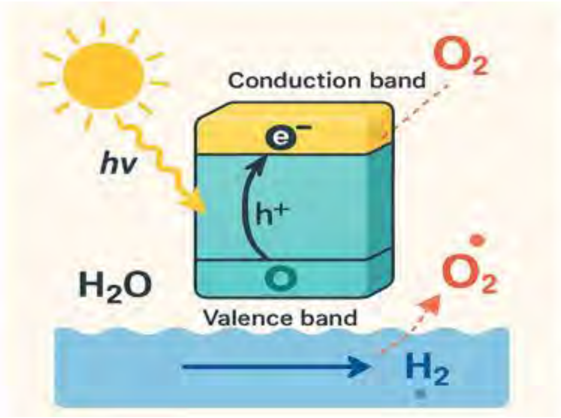
Construction of oxygen deficient NiAl-LDH-nanocomposites for enhanced photocatalytic hydrogen evolution via water splitting

Mametja Sense, Mmelesi Olga[a], *X. Liu*[a], *and Gorimbo Joshua*[a]

[a] Institute for Catalysis and Energy Solutions, College of Science, Engineering and Technology, University of South Africa, Florida Park, 1709 Johannesburg, South Africa; E-mail correspondence: 22469567@mylife.unisa.ac.za

Keywords: Photocatalysis, defects, hydrothermal, chemical reduction, photocatalytic activity.

Recently, hydrogen has received remarkable scientific attention as a renewable resource in energy applications since the current energy production processes include combustion of non-renewable resources, highly contributing to the effect of global warming due to great emission of greenhouse gases [1]. This study addresses the production of hydrogen through photocatalytic water splitting, a cleaner alternative to methods such as gasification and steam methane reformation, which emit a large quantity of carbon dioxide and thus undermining the environmental sustainability goal. Photocatalysis is defined as the enhancement of a photoreaction by employing light as illustrated in **Figure 5**. While several photocatalysts have been explore for hydrogen evolution, this study focuses double-layered hydroxides (LDHs) due to their desirable properties such as distinctive layered structures, cost effectiveness, modifiable compositions, and facile synthesis. However, their large band gap makes it difficult for the promotion of electrons from the valence band to the conduction band, which results in poor photocatalytic activity. To mitigate this, defect engineering (oxygen vacancy) proved to be one of the most efficient techniques to enhance photocatalytic activity [2]. As a cost-effective alternative for platinum (Pt), nickel (Ni) and aluminium (Al) were embedded within LDH to form NiAl-LDH, followed by chemical reduction using different concentrations of sodium borohydride ($NaBH_4$) to construct oxygen vacancy. FTIR, Raman, and XRD showed successful formation of the nanocomposites and reduced peak intensities due to the removal of oxygen. The UV-VIS-DRS spectra and Tauc plots revealed enhanced light absorption capacity as well as reduced band gap energy respectively. Interestingly, the introduction of oxygen vacancies increased the quantity of active sites and reduced Tafel slope, indicating faster reaction kinetics.



Light absorption

$PC + hv \longrightarrow e- + h^+_{vb}$

Oxidation reaction

$2H_2O + 4H^+_{vb} \longrightarrow O_2 + 4H^+$

Reduction reaction

$2H^+ + 2e^- \longrightarrow H_2$

Overall reaction

$2H_2O \longrightarrow 2H_2 + O_2$

Figure 5. Illustration of photocatalytic water splitting for hydrogen evolution.

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Exploring Morphology-Dependent Photocatalysis of ZnO Nanoparticles Towards Rhodamine 6G Degradation Under UV Light

Mbali Moreki[a], *Gold Matlou*[b] *Nomasonto Rapulenyane*[a] *Charmaine Tshangana*[c]

[a] Department of Chemistry and Chemical Technology, Sefako Makgatho Health Sciences University, Molotlegi Street, Ga-Rankuwa, 0204, South Africa, e-mail: 201803688@swave.smu.ac.za. [b] Electron Microscopy Unit, Sefako Makgatho Health Sciences University, Molotlegi street, Ga-Rankuwa, 0204, Pretoria, Gauteng, South Africa, [I]nstitute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Johannesburg 1709, South Africa,

Keywords: Rhodamine 6G, Zinc Oxide nanomaterial, Morphology Control, Surface Defects, Mesoporous Structure and Photodegradation.

This study reports on the synthesis of ZnO nanoparticles with different morphologies using the Sol-Gel method under varying conditions namely; pH, temperature, solvents, and precursors to enhance their photocatalytic properties. The aim of the study was to evaluate how morphological variations influence ZnO's ability [2-3] to degrade Rhodamine 6G (R6G), a complex organic dye pollutant, under neutral pH (7) and visible light.

The Characterization of the nanoparticles was performed using XRD, UV/VIS, FTIR, TEM, BET and SAED. The crystalline size ranged between 20 and 68 nm, determined by the Debye Scherrer equation, with the characteristic Zn-O peaks following the JCPDS card 36-1451, with hkl values: (100), (002), (101), (102), (110), (103), and (112). This was further confirmed by the SAED hkl indices with values (100) (101) (102) (110) (103) (and (112) different for each ZnO NP. The XRD of ZnO-1E that is synthesised under alkaline conditions with citrate used to stabilise it, had shown defects on its surface. The UV Vis spectra revealed absorption bands between 300-370 nm, while FTIR spectra showed characteristic stretching vibrational Zn-O bands between 350 and 400 cm^{-1}. TEM showed quasi-spherical structures with lattice fringes ranging around 0.25 to 0.29 nm and a size distribution range between 20-150 nm with agglomeration causing size to range to 300 nm for the plain ZnO (1C). BET analysis indicated that all ZnO had H3 hysteresis loop and a Type IV BET curve, with a mesoporous structures and surface area ranging from 1.9606, 3.4741, 0.9547, 1.9190 and 8.8739 m^2/g for ZnO-1A to ZnO-1E respectively.
Photocatalytic activity was evaluated by monitoring the degradation of Rhodamine 6G under UV lamp for a duration of 60 minutes. The ZnO NPs (1A (30.35nm), 1B (26.27 nm) and 1D(68.76nm)) had the lowest percent degradation (20% ,27.6 % and 20.7% respectively), while ZnO NPs (1C (32.75 nm) and 1E (20.40 nm)) had the highest percent degradation (70.5% and 83% respectively).The kinetic study of the degradation revealed that ZnO -1A to D followed a pseudo-first order reaction model. Notably ZnO-1E, followed a zero-order kinetic model (ZnO-1E (K=-0.01625, R^2=0.971) and had the shortest half-life of 37 minutes indicating superior photocatalytic efficiency.

According to the findings of the study, the ZnO with the most defects caused by citrate on its surface exuded the highest photocatalytic performance, under neutral conditions simulating the natural environment and UV light.

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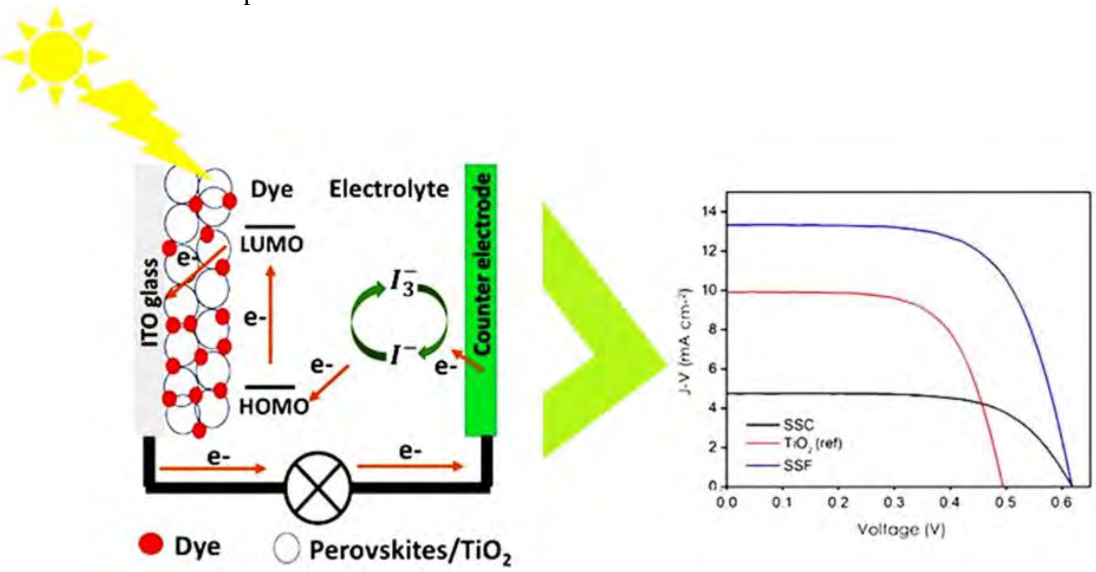
Enhancing dye-sensitized solar cell performance by introducing Fe/Co into the B-site of $Sr_{0.7}Sm_{0.3}BO_{2.89}$ perovskite photoanodes

Samantha Ndlovu, Edigar Muchuweni and Vincent O. Nyamori

[a] School of Chemistry and Physics, University of KwaZulu-Natal, Westville Campus, Private Bag X54001, Durban, 4000, South Africa, E-mail: ndlovus4@ukzn.ac.za.

Keywords: perovskites, dye-sensitised solar cells, photoanode, photovoltaics

The desire for clean, affordable, and efficient energy technologies that can harvest light to generate electricity has led to recent developments in new-generation solar cells. Among them, dye-sensitized solar cells (DSSCs) have numerous merits, including low impact on the environment, facile fabrication procedures, and the associated low cost of raw materials. However, the power conversion efficiency (PCE) of DSSCs is limited by poor electron injection and high charge carrier recombination in conventional photoanode materials. This, in turn, has prompted significant research efforts to find alternative photoanode materials. In this study, we report a novel perovskite-based photoanode material ($Sr_{0.7}Sm_{0.3}BO_{2.89}$) optimised by varying the B-site using Fe or Co. To achieve this, $Sr_{0.7}Sm_{0.3}FeO_{2.89}$ (SSF) and $Sr_{0.7}Sm_{0.3}CoO_{2.89}$ (SSC) perovskites were synthesised using the ball milling method, calcined at 600 °C, and characterised using various techniques. Varying the B-site using Fe or Co significantly influenced the structure and morphology of $Sr_{0.7}Sm_{0.3}BO_{2.89}$. Both perovskites revealed the formation of irregularly shaped nanoparticles with cubic and tetragonal lattices for SSF and SSC, respectively. SSF, with relatively smaller particle sizes, larger pore volumes, and better crystallinity, exhibited a relatively larger surface area (52.6 m^2 g^{-1}), lower energy band gap (2.4 eV), and higher electrical conductivity (4.98 S cm^{-1}) than SSC. This led to the fabrication of SSF photoanode-based DSSCs with an enhanced PCE of 6.24%, outperforming SSC-based devices by ~109%. Therefore, this study demonstrates that varying the B-site cations can significantly improve the physicochemical properties of perovskites for use as photoanodes in future DSSCs.



Moringa Oleifera and *Marula*-derived platforms for bioanalytical and biomedical applications

Nare Leah Mojela[a], *Kriveshini Pillay*[b], *Pradeep Kumar*[b], *Yahya Choonara*[b], *Raveen Parboosing*[b], *and Patrick Komane*[a]

[a] Department of Chemical Sciences, Faculty of Science, University of Johannesburg, P.O. Box 17011, Doornfontein 2028, Johannesburg, South Africa, Email: nareleah02@gmail.com. [b]Department of Pharmacy and Pharmacology, Faculty of Health Science, University of the Witwatersrand,7 York Road, Parktown, 2193, Johannesburg, South Africa

Keywords: AuNPs, AgNPs, body fluids, plant extracts, exosomes, H1N1

A key aspect of forensic investigation involves identifying and detecting body fluid stains, preserving them for subsequent DNA extraction, and identifying the right criminals. Body fluid stains frequently encountered at a crime scene are blood, urine, saliva, etc. The process of stain identification might provide challenges due to the limitations of current techniques, which are primarily focused on certain body fluids and often involve destructive procedures. Chemical reagents such as luminol and DMAC are primarily used for detecting body fluids at crime scenes. However, these chemicals have limitations like short shelf life, lower specificity, and sensitivity. To address these concerns, alternate materials derived from extracts of *Marula* and *Moringa* stems were used in this project to provide a universal, confirmatory, and non-invasive methodology capable of identifying and distinguishing various bodily fluids. Silver and gold nanoparticles from these plants were used to enhance the performance of Luminol and DMAC to be more sensitive and specific to a specific fluid stain. Promising results were discovered from this project. Furthermore, the nanoparticles were assessed for their antiviral efficacy against the influenza virus. HEK 293 cells were infected with H1N1, a strain known for its pandemic potential. The treatment utilized exosomes sourced from *Moringa* alongside gold nanoparticles. Cytotoxicity and cellular uptake studies indicated that lower concentrations of AuNPs preserved cell viability, whereas higher doses reduced it. Cellular uptake studies validated nanoparticle internalization. The properties of metal nanoparticles and exosomes were verified through characterization techniques, including TEM, HRSEM, FTIR, XRD, etc.

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From leaves to leads: Uncovering potential COX-2/5-LOX dual inhibitors from South African medicinal plants

Tatenda Machakaire, *Fanie R. van Heerden, and Muvhango Rasalanavho*

[a] School of Agriculture and Science, Discipline of Chemistry, University of KwaZulu-Natal, Pietermaritzburg, South Africa, Email: 21700136@stu.ukzn.ac.za

Keywords: Inflammation, COX-2 inhibition, 5-LOX inhibition, dual inhibition, medicinal plants

Chronic inflammation disrupts immune homeostasis and contributes to the pathogenesis of various diseases. While conventional non-steroidal anti-inflammatory drugs (NSAIDs) primarily target cyclooxygenase (COX) enzymes to relieve symptoms, selective COX inhibition can divert arachidonic acid metabolism towards the LOX pathway, which can lead to adverse effects. The dual inhibition of COX and LOX pathways has therefore emerged as a more balanced therapeutic approach [1].

South Africa's rich ethnomedicinal heritage includes nearly 495 plant species traditionally used to treat pain and inflammation [2]. Although crude extracts from several of these plants exhibit measurable anti-inflammatory effects [3], the specific bioactive compounds remain largely unknown. This study investigates the potential of South African flora as a source of novel dual COX-LOX inhibitors. We identified candidate plant species with reported COX-2 and/or 5-LOX inhibitory activity, evaluated experimental methodologies, and analyzed compounds potentially responsible for the observed bioactivity. Data were compiled from ethnobotanical records, in vitro assays and in silico modelling, and compound-level studies [4]. Species within the Anacardiaceae and Meliaceae show consistent extract-level inhibition, although the direct translation to compound-level activity remains unclear.
To account for variation in extract concentration and assay conditions, potency was normalized using mathematical equations. An Anti-inflammatory Index (AI index) was developed from inhibition data for COX-1, COX-2, and 5-LOX, highlighting promising dual inhibitors. Docking simulation of previously isolated compounds revealed molecular interactions consistent with anti-inflammatory activity. By integrating traditional knowledge with pharmacological evaluation, this work provides a framework for the discovery of accessible, plant-derived therapeutics targeting dual COX-LOX inhibition (**Figure 1**).

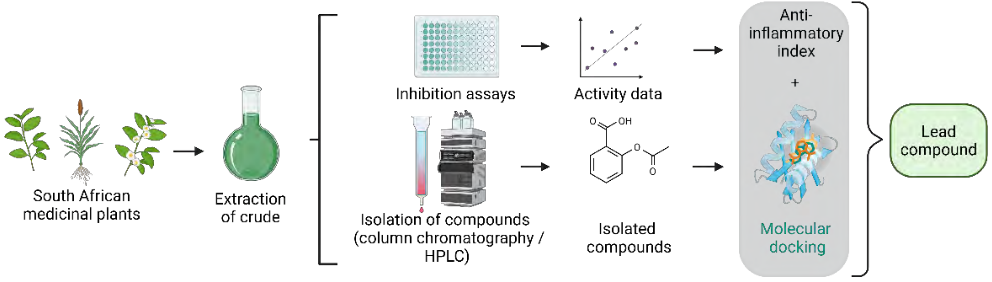

Figure 1. A systematic approach to identifying COX-2/5-LOX inhibitors in medicinal plants.

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Innovative Inner Transition Metal-MXene Anodes for High Performance Sodium-ion Batteries

Feleni Gwibakazi, Miranda Ndipingwi and Emmanuel Iwuoha

[a] SensorLab (University of the Western Cape Sensor Laboratories), 4th floor Chemical Sciences Building, University of the Western Cape, Robert Sobukwe Road, Bellville 7535, Cape Town, South Africa. E-mail: 4427938@myuwc.ac.za

Keywords: Anode materials, Electrochemical performance, Hydrothermal synthesis, Lanthanide-doped MXene, Sodium-ion battery

Sodium-ion batteries (SIBs) are widely explored as cost-effective alternatives to lithium-ion batteries due to their low cost and abundance of sodium resources. However, their performance is often limited by the sluggish kinetics and volume changes caused by the large Na^+ radius. To address this, we developed lanthanide-doped Ti_3C_2 MXene as a promising anode material with improved sodium storage behaviour. Few layered Ti_3C_2 MXene was synthesized from Ti_3AlC_2 MAX phase using a hydrothermal etching process with fluoride containing acidic solution to remove the Al layer. X-ray diffraction (XRD) confirmed the successful transformation from MAX phase to MXene and revealed a shift in the (002) peak after doping, indicating increased d spacing and X-ray photoelectron spectroscopy (XPS) verified the presence La^{+3} and Gd^{+3} on the MXene surface along with changes in Ti oxidation states. To further enhance its electrochemical properties, varying ratios of La^{3+} and Gd^{3+} ions were introduced through a wet chemical doping method using $La(NO_3)_3.6H_2O$ and $Gd(NO_3)_3.6H_2O$. The incorporation of these rare-earth dopants led to expanded interlayer spacing and increased defect density, which facilitated ion transport and provided more active sites for Na^+ intercalation. Electrochemical testing in 1 M Na_2SO_4 electrolyte showed clear improvements in performance. Gd-doped Ti_3C_2 delivered a specific capacitance of 312 mAh g^{-1} at 100 mA g^{-1}, while the La-doped MXene reached 278 mAh g^{-1} under the same conditions. Even at 1000 mA g^{-1}, over 70% of the initial capacitance was retained indicating high-rate capability. Long-term cycling over 2000 cycles at 500 mA g^{-1} resulted in 91% capacity retention for the Gd-doped electrode. Impedance measurements also revealed a low charge-transfer resistance of 1.8 Ω, suggesting improved electronic conductivity and ion diffusion. The improved sodium storage performance is attributed to the synergistic effect of rare-earth doping, which modify the surface chemistry, improves conductivity, and increases interlayer spacing. This study highlights a simple and scalable strategy for designing doped MXene-based anode materials with tunable properties for next-generation sodium-ion batteries.

Hybrid Bifunctional FeCo-Fe_2CoO_4 electrocatalyst Anchored on Carbon Support for High Areal Energy Rechargeable Zinc-Air Battery.

Augustus K. Lebechi, Agnes M. Mongwe, Aderemi B. Haruna, and Kenneth I. Ozoemena

[a] Molecular Science Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Johannesburg, 2050, South Africa, E-mail: 2787681@students.wits.ac.za

Keywords: Oxygen evolution reaction, oxygen reduction reaction, Rechargeable Zinc-air battery

The development of rechargeable zinc-air batteries has been hampered by the slow kinetics of the oxygen evolution and oxygen reduction reactions occurring concurrently in the air cathode. Hence, rational design of robust, bi-efficient and cost-effective electrocatalysts is necessitated. Herein, we report on the novel hybrid bifunctional electrocatalysts FeCo-Fe_2CoO_4 confined in Vulcan XC-72 carbon as support and synthesized via a facile annealing alone (FeCo-Fe_2CoO_4/C_{Ann}) and microwave-assisted annealing (FeCo-Fe_2CoO_4/C_{MW}) procedures. The electrocatalyst synthesized via the annealing procedure alone showed better OER and ORR performance in terms of charge/electron transfer kinetics as revealed by the bifunctionality index ($\Delta E = 0.76$ V vs RHE) which is lower than that obtained for FeCo-Fe_2CoO_4/C_{MW} ($\Delta E = 0.84$ V vs RHE) and even matches that obtained for 20 wt% Pt/C-IrO_2 ($\Delta E = 0.75$ V vs RHE). This result was corroborated by the smaller value obtained for the Tafel slope for FeCo-Fe_2CoO_4/C_{Ann} (45 mV dec^{-1}) compared to the (59 mV dec^{-1}) value obtained for FeCo-Fe_2CoO_4/C_{MW}. In a proof-of-concept, FeCo-Fe_2CoO_4/C_{Ann} was employed as the air-cathode electrocatalyst for RZAB constructed in a micro-3D-printed cell configuration. The fabricated RZAB showed a high peak power density of 146.12 $mWcm^{-2}$, superior specific capacity 690 $mAhg^{-1}{}_{zn}$ compared to that from RZAB fabricated with Pt/C+IrO_2 as the air cathode (421 $mAhg^{-1}{}_{zn}$), superior area-discharge energy (≥ 48 mW h/cm^2) and cycling stability (~ 8 cycles at 8 h per cycle for 65 h at 10 mA cm^{-2}), maintaining a stable discharge voltage of ~1.2 V. The RZAB fabricated with FeCo-Fe_2CoO_4/C_{MW} as the air cathode showed deterioration in the discharge voltage after the 1st cycle when cycled at 8 h and 10 mA cm^{-2}. This result shows that oxidizing the alloy component by microwaving greatly compromised the stability of the catalyst. Hence, the superior performance of FeCo-Fe_2CoO_4/C_{Ann} can be attributed to its higher alloy content and improved synergy between the alloy and oxide components. Therefore, this work brings the synergistic effects of alloys and oxides together for improved rechargeable zinc-air battery.

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Investigation of high entropy manganese-based fluorophosphate electrocatalysts for electrocatalytic and energy storage applications

Aderemi B. Haruna, Lesego Gaolatlhe, Dean Barrett and Kenneth I. Ozoemena

[a] Molecular Science Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Johannesburg, 2050, South Africa, E-mail: aderemi.haruna@wits.ac.za

Keywords: manganese fluorophosphate, Electrocatalysts, energy storage, high-entropy

High-entropy materials are emerging electrocatalytic and energy storage technology materials that have gained significant interests due to their unique structure, complex stoichiometry and corresponding synergetic effect. Even with the increasing number of published articles on high-entropy materials over the years, there are still rare reports on the details of their structural properties in relation to their electrochemical performances. Therefore, this study investigates the design, synthesis, structural properties in relation to the electrochemical performances of $Mn_2(PO_4)F$, $Co_{0.4}Cu_{0.4}Fe_{0.4}Mn_{0.4}Ni_{0.4}(PO_4)F$ and $Co_{0.25}Cu_{0.25}Fe_{0.25}MnNi_{0.25}(PO_4)F$ electrocatalysts. The electrocatalysts are thoroughly characterized using different techniques including high-resolution transmission electron microscopy, field-emission scanning electron microscopy, Raman spectroscopy, powder neutron diffraction, X-ray photoelectron spectroscopy, synchrotron X-ray diffraction, and electrochemistry. The findings in this research work present unique possibilities for manipulating the structure–property relationships in high entropy manganese-based fluorophosphate electrocatalysts for electrocatalytic and energy storage applications.

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Investigations into emissions from domestic solid waste burning

Neale Berkenbosch[a], *Alexandra de Vos*[b,c] *and Patricia Forbes*[a]

[a]Department of Chemistry, University of Pretoria, Lynnwood Road, Pretoria, 0002, South Africa, E-mail: neale.berkenbosch@tuks.co.za.
[b]Department of Chemical Engineering, University of Pretoria, Lynnwood Road, Pretoria, 0002, South Africa.
[c]Sasol Research and Technology, 1 Klasie Havenga Road, Sasolburg, Free State, 1947, South Africa.

Keywords: domestic waste burning; polycyclic aromatic hydrocarbons; gaseous emissions

Open burning of domestic solid waste is a widespread practice in South Africa largely due to limited or inconsistent waste collection services. This leads to the emission of numerous pollutants—including polycyclic aromatic hydrocarbons (PAHs), SO_2, volatile organic compounds (VOCs), particulate matter with aerodynamic diameter less than 2.5 µm ($PM_{2.5}$), and nitrogen oxides (NO_x)—which pose health risks to communities as well as contributing to broader environmental pollution. This study determined targeted gas-phase PAHs emitted from domestic waste burns in a South African community, and concurrently measured $PM_{2.5}$, SO_2, VOCs, and NO_x using portable continuous sensors. Temperature profiles of the burns were captured with a thermal imaging camera. Low-molecular-mass ($\leq$ 202 $g \cdot mol^{-1}$) gas-phase PAH concentrations ranged from 1.3 to 8.7 $\mu g \cdot m^{-3}$ in smoke plumes, while time-averaged $PM_{2.5}$ concentrations ranged from 323 (± 283) to 1368 (± 592) $\mu g \cdot m^{-3}$. Temporal variation in pollutant concentrations and temperature profiles revealed substantial variability in emissions, emphasising the need for representative environmental sampling. This study highlights the need for education regarding the potential health risks of domestic waste-burning, and supports the call for improved waste management services.

Investigation into the odour contributions from a hazardous waste management facility and surrounding sources using TD-GCxGC-ToFMS

Thea Smuts, Yvette Naudé and Patricia Forbes[a]

[a]Department of Chemistry, University of Pretoria, Faculty of Natural and Agricultural Sciences, Pretoria, 0002, South Africa, E-mail: thea.smuts@tuks.co.za.

Keywords: odour forensics, thermal desorption, gas chromatography-mass spectrometry, air quality

Odorous emissions from hazardous waste management facilities pose environmental and community challenges. This study explores how advanced chemical analysis can be used to understand and manage such emissions using polydimethylsiloxane multichannel traps to collect volatile and semi-volatile organic compounds in air sampled seasonally. Chemical fingerprints of the sampling sites were established by means of thermal desorption-comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (TD-GC×GC-ToFMS). Preliminary analyses indicate clear chemical grouping patterns, with hydrocarbons (e.g. nonane), nitrogen-containing compounds (e.g. pyridine), and ketones (e.g. cyclohexanone) associated with specific site activities and meteorological conditions. This study advances a quantitative framework for improved odour source apportionment, supporting more effective odour diagnostics and monitoring for air quality management. Ultimately, it demonstrates how chemistry can drive meaningful environmental change and bridge industrial activity with community well-being.

Phytochemistry and biological studies of selected medicinal plants

O Adebayo[a], CP Anokwuru[b], IDI Ramaite[a], and D Tlhapi[a]

[a] Department of Chemistry, University of Venda, Thohoyandou, South Africa,
[b]Department of Basic Sciences, School of Science and Technology, Babcock University, Nigeria
Email: Isaiah.Ramaite@univen.ac.za

Keywords: *Phytochemistry, Isolation, Bioactive compounds, Metabolomics.*

The Vhembe region, Limpopo province, has a very rich biodiversity of a wide range of plants which are currently being exploited by traditional health practitioners for the treatment of various communicable diseases such as TB, HIV, and influenza; and non-communicable diseases such as diabetes, cancer, malaria, etc. Our natural products research team has been working on different plants such as *Terminalia sericea, Rauvolfia caffra, Breonadia Salicina, Melia azedarach, etc.*

Terminalia sericea Burch ex. DC. Ethno medicinal information revealed that the fruit, leaves, stem bark and roots of *T. sericea* are commonly used for the treatment of coughs, skin infections, diabetes, diarrhea, and gonorrhoea. The chemical profiles and antibacterial activities of several root bark samples were collected and evaluated, withn nine compounds isolated from the root bark.[1,2] *Rauvolfia caffra* Sond, used for the treatment of malaria, diabetes, coughs, etc was also investigated. Phytochemical studies revealed that indole alkaloids are the major constituents of the stem bark. Our research also investigated *Melia azedarach*. Bioactive metabolites such as epicatechin and catechin were isolated and displayed good antiplasmodic activity.[3,4]
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Nano-encapsulation strategies for enhancing stability, bioavailability and therapeutic potential of fucoxanthin

Witness Sibiya, *Denzil R. Beukes and Edith A. Beukes*

[a]Department of pharmacy, University of the Western Cape, Bellville, Cape Town, 7535, South Africa, E-mail: 4493945@myuwc.ac.za [b]Department of Biomedical Sciences, University of the Western Cape, Bellville, Cape Town, 7535, South Africa

Keywords: Fucoxanthin, Nanotechnology, Bioavailability, Stability, Lipophilic

Fucoxanthin, a carotenoid produced from marine brown algae, has received interest in its potential medicinal characteristics, which include antioxidant, anti-inflammatory, and anticancer activities. However, its lipophilic nature restricts its solubility and bioavailability, making it unsuitable for drug delivery applications. To address these constraints, this study will design and test nano-encapsulation techniques for fucoxanthin. This work aims to improve the solubility, stability, and cellular absorption of fucoxanthin by encapsulating it in lipid-based , hence increasing bioavailability and therapeutic potential. To examine the qualities and efficiency of these nanoformulations for this study, Fucoxanthin was extracted from a South African marine brown Algae called Sargassum folicium and isolated, followed by synthesis and nano-encapsulation of lipid-based nanoparticles using hot homogenizing technique. Sophisticated and advanced analytical characterization techniques such as NMR and UV-Vis spectroscopies, as well as Dynamic Light Scattering (DLS) and SEM were used to characterize and visualize the nanoformulations. The nano formulations were further taken for microbial studies. Notably, antimicrobial assays and they are expected to show strong inhibition of Gram-positive bacteria by the encapsulated fucoxanthin, consistent with its reported antibacterial potential. The nanoparticles resulted in increased solubility, stability and bioactivity, thereby boosting fucoxanthin as a viable option for a variety of therapeutic uses. The results demonstrated that nano-encapsulation not only improves the physicochemical properties of fucoxanthin but also broadens its functional scope. This research might open the way for more efficient use of marine bioactive chemicals in the pharmaceutical and nutraceutical sectors.

Comparison of soxhlet and microwave assisted extractions efficiency for the determination of herbicides in soil and maize cob: cumulative and health risks assessment

Sandisiwe Zondo[a], *Precious Mahlambi*[b*]

[a]KwaZulu-Natal Department of Agriculture and Rural Development, PBag X6005, Hilton, 3245, South Africa
b*Department of Chemistry, University of KwaZulu Natal, PBag X01, Scottsville, Pietermaritzburg, 3209, South Africa

Keyword: Health risk index; MAE; Maize Maximum limits; Pesticide toxicity index; Soxhlet

The effectiveness of microwave-assisted extraction (MAE) and Soxhlet extraction (SE) was compared for the determination of herbicides (atrazine, 2,4-D, mesotrione and glyphosate) in soil and maize crop followed by gas chromatography with flame ionization detector. The recoveries of herbicides in maize and soil were 62-80% and 70-81%, respectively for SE, while they were 80-98% and 85-101%, respectively for MAE. The analysis repeatability, represented as relative standard deviations were less than 20% for all herbicides in both methods. All the herbicides calibration curves showed a good correlation coefficient (R^2) $\geq$0.996, indicating good linearity. The SE limits of detection and quantification ranged between 0.22-0.32 µg L^{-1} and 2.2-3.2 µg L^{-1}, respectively, while they were between 0.1-0.29 µg L^{-1} and 1.0-2.9 µg L^{-1}, respectively for MAE. These findings showed that MAE method is more accurate and sensitive than SE, thus can be accurately applied for the determination of the assessed herbicides in soil and maize cop. Herbicides concentrations obtained ranged from 2.7 – 20.4 µg L^{-1} in maize and 1.2 - 30.5 µg L^{-1} in soil samples. The concentrations obtained in maize were higher than the maximum residue limits suggesting that health effect may occur upon continuous consumption. The herbicides toxicity index further confirmed the possible high toxicity effect of the studied maize crop as it exceeded the threshold value of 1. However, the health risk index was lower than 100% limit and did not exceed the acceptable daily intake of the maize crop in both adult and children indicating no health effect.

Possible value recovery of rare earth elements and other valuable elements from acid mine drainage resulting from closed and abundant mines in Krugersdorp

Mildred M. Phasha[ab], *Matthys A. Dippenaar* [b] , *Zakhele H. Nkosi*[b] *and Alseno K. Mosai* [a]

[a]*Department of Chemistry, University of Pretoria, Lynwood Road, Pretoria, 0002, South Africa, E-mail:* *u21764906@tuks.ac.za*.
[b]*Department of Geology, University of Pretoria, Hatfield campus, Pretoria, 0002, South Africa*

Keywords: rare earth elements, toxic elements, acid mine drainage, recovery technique

The present study focused on identifying and quantifying valuable elements (e.g., rare earth elements (REEs)) that can be recovered from waterbodies and sediments around closed and abandoned gold mine dumps in Krugersdorp, Gauteng Province, South Africa. Solid and liquid samples were collected and gathered for analysis. Physiochemical parameters such as temperature, pH, conductivity, colour, redox potential and TDS were measured and the water was found to be acidic (pH 3), with high levels of dissolved substances. Solid samples were digested using a mixture of HCl, H_2SO_4 and HNO_3 after drying at room temperature for 7 days and oven drying at 80 ˚C for 4 hours. Analytical methods such as Inductively coupled plasma optical emission spectroscopy (ICP-OES) was used for elemental analysis, Fourier transform infrared spectroscopy (FTIR) for functional group identification, and Brunner-Emmett-Teller (BET) for surface area and pore size analysis.

Higher concentrations of REEs and valuable elements were found in solid samples compared to water, likely due to strong soil binding sites. Liquid REEs concentrations ranged from 0-2 mg/L, with Ce and Te being the most prevalent, while base metals like Al, Fe, Zn, and Ni presented higher concentrations (5- <180 mg/L). Toxic elements such as Pb, Cr, Tl, In and Cd exceeded World Health Organisation (WHO) limits, along with high concentrations (>10 mg/L) of Ag, Co, Li, and Mn [1]. Solid and liquid samples exhibited different infrared spectra indicating varying compositions, with specific absorbance peaks attributed to carbonyl and hydroxyl groups in liquids and C-H, C-O bonds in solids [2]. The soil was characterized as microporous with low surface area due to large soil particles which resulted in few contact points. The results suggest that the study area holds potential for recovering REEs and other valuable elements from secondary sources impacted by mining activities.

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Structure-property relationships in recycled agricultural netting

Karabo P Lehabe[a], *Megan E Matthews*[b]

[a]Department of Chemistry & Polymer Science, Stellenbosch University, Stellenbosch, 7600, South Africa, E-mail: 21025606@sun.ac.za.

Keywords: polyethylene, agriculture, recycling, netting

Netting and permeable covers find far-reaching applications in the agricultural industry for protection of crops from insects and weather elements. When used for these purposes, the nets facilitate the use of less agrochemicals or pesticides. In addition, netting also provides an insulating effect and can provide partial shade in greenhouses, reducing some energy costs. They can therefore enhance both the quantity of produce as well as the quality of the crops by regulating the local microclimate in the crop space[1]. Due to the environmental application of these nets, the required composition should be highly resistant to environmental degradation. For this reason, high density polyethylene (HDPE) is a popular polymer for agricultural permeable covers.

Traditional HDPE is highly crystalline and very rigid, and the resultant nets may suffer from embrittlement during the lifecycle of the net. Modern net compositions have evolved to use bimodal HDPE which contains two molecular weight distributions. This provides the net structure with additional strength in addition to the environmental stress-crack resistance of conventional HDPE[2]. New regulations on extended producer responsibility (EPR) require net producers and raw material suppliers to manage net waste after its lifecycle ends. To facilitate circular economy practices within the agricultural industry, these nets should be recycled into a second lifecycle. This project addresses this issue by investigating the recycling potential of agricultural nets in the industry. The project involves blending old nets after different durations of environmental exposure from the Limpopo and the Western Cape provinces of South Africa with varying ratios of virgin HDPE polymer to study their structure-property relationships for recycling potential. Net samples will be studied from farms in different climate regions in South Africa with varying exposure times and characterized in terms of degradation levels. Pesticide concentrations will also be evaluated as a potential hazard during the recycling process.

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Exploring South African honey: a focus on chemical composition and antimicrobial activity against pathogenic organisms

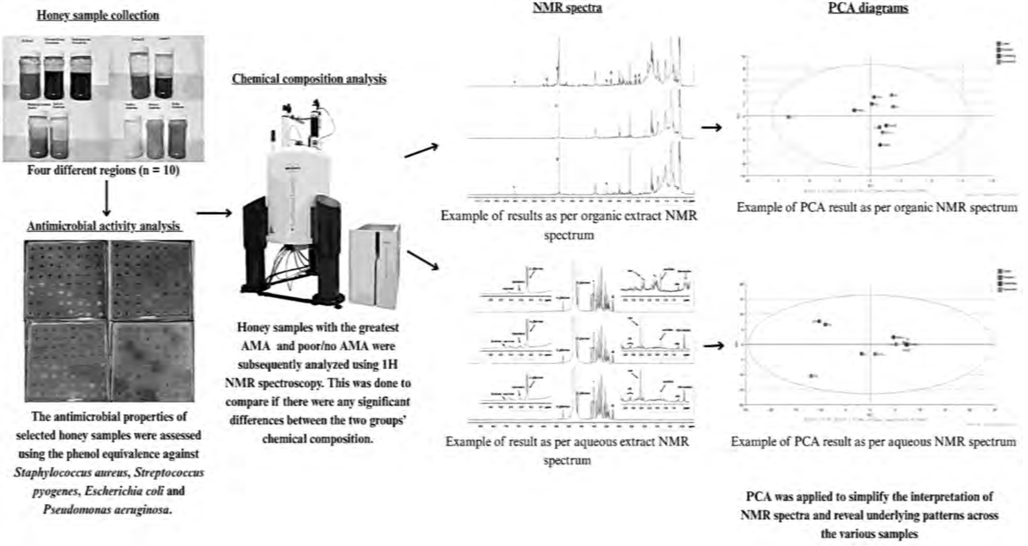
Tanya Rohman[a], *Pedro M.D.S. Abrantes*[a], *Mike Allsopp*[b], *Retha C.M. Kotze*[c] *and Edith Antunes*[d]

[a] Department of Medical Biosciences, University of the Western Cape, Robert Sobukwe Rd, Bellville. 7535, South Africa, E-mail: 3940349@myuwc.ac.za. [b] Honey Bee Research Section, Agricultural Research Council - Plant Health & Protection Research Institute, Stellenbosch, South Africa. [c] Department of Dietetics and Nutrition, University of the Western Cape, Robert Sobukwe Rd, Bellville. 7535, South Africa. [d] Department of Chemistry, University of the Western Cape, Robert Sobukwe Rd, Bellville. 7535, South Africa

Keywords: South African honey, antimicrobial activity, chemical composition, NMR

The introduction of antibiotics marked a breakthrough in the fight against life-threatening infections, but unfortunately, because of the widespread use thereof, antimicrobial resistance emerged not long after [1, 2]. This growing concern stresses the urgent need to explore alternative ways to treat infections. An organic product that has gain attention over time is honey. While prior research focused on South African honey, its antimicrobial potential and the chemical composition remains largely underexplored [3]. The aim of this study is therefore to identify South African honey that exhibits exceptional antimicrobial activity (AMA) against selected pathogenic microorganisms.

The study design is presented below (Figure 1). The AMA results showed that samples from the Namaqualand and Overberg regions had exceptional AMA against the four bacterial organisms whereas samples from the Sandveld region, demonstrated the weakest AMA. Although the Principal Component Analysis (PCA) indicated some regional differences in floral types, the ^{1}H NMR analysis suggests that such variations may not have significantly contributed to the overall AMA observed. However, other mechanisms such as hydrogen peroxide activity, sugar content and proteinaceous compounds could be responsible for the honey samples with a high AMA.



The antimicrobial properties of selected honey samples were assessed using the phenol equivalence against *Staphylococcus aureus*, *Streptococcus pyogenes*, *Escherichia coli* and *Pseudomonas aeruginosa*.

Honey samples with the greatest AMA and poor/no AMA were subsequently analyzed using 1H NMR spectroscopy. This was done to compare if there were any significant differences between the two groups' chemical composition.

PCA was applied to simplify the interpretation of NMR spectra and reveal underlying patterns across the various samples

Figure 1: Schematic diagram of the study design.

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Chemical characterization of *Amaranthus hybridus* leaf extract as a potential biostimulant

Vanessah Lekalakala[a], *Luke Chimuka*[a] *and Nkazimulo Ngwenya*[a]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa

Keywords: Amaranthus hybridus, biostimulant, phytochemicals

Food security is one of the world's biggest issues currently. It does not just encompass the availability of food, but the accessibility and nutrition adequacy. Risks posed by climate change, population increase, soil degradation, water scarcity and unsustainable farming practices have further impacted on meeting global food demands as the world's population is expected to reach fifty billion people by 2050. Techniques to mitigate these challenges include the use of biostimulants in agricultural sectors. Biostimulants are substances that promote resistance to biotic and abiotic stress and enhance nutrient uptake. They are derived from various sustainable sources, including terrestrial plant extract, rich in phytochemicals. Amaranthus hybridus, also known as smooth amaranth, is one such plant valued for its nutritional and medicinal properties. It is rich in phytochemicals such as phenolics, flavonoids, tannins and betalains, making it a sustainable candidate for biostimulant production. The aim of this study to extract phytochemical from Amaranthus hybridus leaves using PHWE and to characterize phytochemicals and metal content of the extracts for potential biostimulant use. Total phenolic content, total flavonoid content and antioxidant activity, determined using Folin-Ciocalteu, aluminum chloride calorimeter and DPPH assays, respectively. Metal concentrations quantified using ICP-OES. Expected results include high levels of phenolic and flavonoid compounds and notable antioxidant activity, along with acceptable concentrations of essential micronutrients and low levels of metals. It is anticipated that these finding will support the potential of Amaranthus hybridus leaf extract as an effective and sustainable plant based biostimulant, contributing to improved crop productivity and resilience.

Exploring the potential of *Lippia javanica* as sustainable bio-adsorbents for removing heavy metals in waste water

Fathima Ndlovu [a], *Precious Mahlambi* [a], *Sihle Mngadi* [b] *and Sandisiwe Zondo* [c]

[a] Department of Chemistry, University of KwaZulu Natal, Pietermaritzburg,3209, South Africa, E-mail: 221004783@stu.ukzn.ac.za. [b] Department of Scientific Services, Laboratories, Chemical Science, Umgeni Water, Pietermaritzburg, 3201, South Africa [c] Department of Agriculture and Rural Development, Howick, 3245, South Africa

Keywords: bio-adsorbents, heavy metals, *Lippia javanica*, sustainable water treatment

Access to clean and safe water is becoming a pressing concern due to increasing anthropogenic activities such as mining, urbanization, and industrialization, which contribute to the persistent rise of water pollution, including heavy metals [1]. While various methods are employed to remove heavy metals from wastewater, they possess inherent drawbacks, including high operational cost and production of toxic sludge [2]. This work explored *Lippia javanica* plant leaves as an alternative biosorbent for heavy metals from wastewater. The effects of pH, contact time, metal concentration, and temperature on copper, zinc, and lead sorption efficiency were investigated through batch experiments. The removal % of 80-99% was achieved within a contact time of 10 minutes. Equilibrium adsorption data were best fitted with the Langmuir isotherm for Cu, and the Freundlich isotherm for Zn and Pb did not conform to any of them. The pseudo-second-order model describes metal adsorption kinetics well. The adsorption capacities of raw, acid, and base-modified *Lippia javanica* material are compared, and the modified composite was found to have greater adsorption capacity. The reusability of the sorbents indicates their effectiveness and stability over multiple cycles of repeated adsorption.

Bio-adsorption has emerged as an environmentally friendly and cost-effective method for removing heavy metals from aqueous solutions.

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Photocatalytic degradation of tetracycline on $MoSe_2$ photocatalyst

Tumisang Lekgetho[a], *Mabuatsela V Maphoru*[a], *Letlhogonolo F Mabena*[a], *and Matshawandile Tukulula*[b]

[a]Department of Chemistry, Tshwane University of Technology, 175 Nelson Mandela Dr, Pretoria, 0001, South Africa, E-mail: maphorum@tut.ac.za. [b]School of Chemistry and Physics, University of KwaZulu Natal, Durban, 4001, South Africa

Keywords: pollutants, semiconductors, photocatalysts, tetracycline

Water pollution caused by innumerate hazardous organic pollutants has become a serious issue in recent years. These pollutants are uncontrollably released into the water environment including toxic chemicals from industries such as pharmaceutical and agriculture [1]. Amongst these contaminants, antibiotics have surfaced as one of the most prevalent pollutants that contribute enormously to the contamination of both surface and groundwater [2]. Owing to their inherent stability, low environmental quantities and high toxicity, these pollutants are often resistant to traditional water treatment methodologies such as adsorption processes and ion exchange and therefore posing the risk of irrevocable harm to human and animal health as well as aquatic life [3]. For example, long term exposure to tetracyclines (TC) has been associated with the destruction of skeletal muscle and cardiomyocyte tissues of adult zebrafish, renal failure, and intracranial hypertension [4]. This necessitates for the design of new, efficient and sustainable technologies. Semiconductor photocatalysis has emerged as an alternative method for the degradation of TC owing to their several advantages such as complete removal of TC and its derivatives, as well as high degradation efficiency. In this work the effect of catalyst dose on the photodegradation of tetracycline was carried out using $MoSe_2$ photocatalyst under UV irradiation using 10 ppm at pH 4 and room temperature. The catalyst was prepared by hydrothermal method and its physicochemical properties were examined using XRD (Figure 1a). The highest degradation efficiency of TC was 97.7% achieved at 50 mg of catalyst, while 96.7% and 94.0% efficiencies were achieved at 20 mg and 35 mg, respectively.

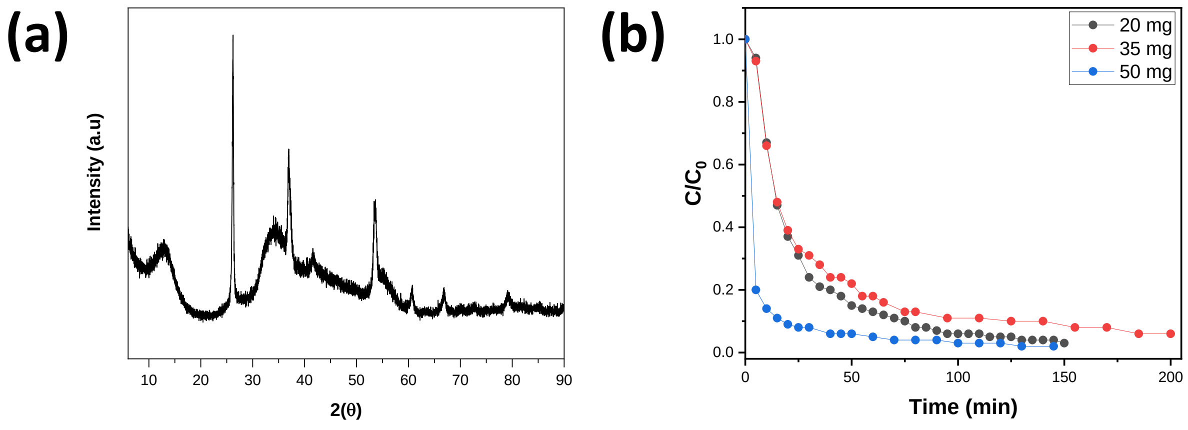

Figure 1: XRD patterns of $MoSe_2$ (a), photodegradation of tetracycline under UV light at varying catalyst dosages.

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Phytochemistry and chemical profiling of *Combretum zeyheri* for management of crop diseases

RM Mathole[a], MF Mashigo[a], VJ Tembu[a]

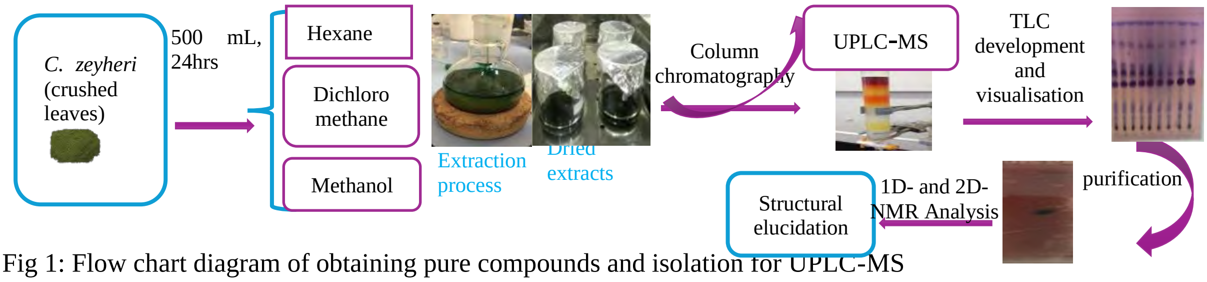
[a]*Department of Chemistry, Faculty of Science, Tshwane University of Technology, Private Bag X680, 175 Nelson Mandela Drive, Arcadia, Pretoria 0001, South Africa, E-mail:* mmatselengmathole@gmail.com

Keywords: phytochemistry, chemometrics, crop pathogens and structural elucidation

Introduction

Infectious plant diseases pose a major threat to global agriculture, causing significant crop losses. It is estimated that 20% to 40% of global crop production is lost annually to pests and diseases, leading to high economic losses [1]. While chemical fungicides and bactericides are effective for high yields in agriculture, their long-term use poses environmental and health risks, including pollution and accumulation in crops, with links to serious health conditions such as cancer [2]. This research aimed to extract, isolate, and identify pure compounds of *Combretum zeyheri* and investigate the chemical profiles of extracts by UPLC-MS. The isolates will then be tested for potential as effective and safer alternatives for control of crop pathogens.

Methodology



C. zeyheri (crushed leaves)

500 mL, 24hrs

Hexane

Dichloromethane

Methanol

Extraction process

Dried extracts

Column chromatography

UPLC-MS

TLC development and visualisation

purification

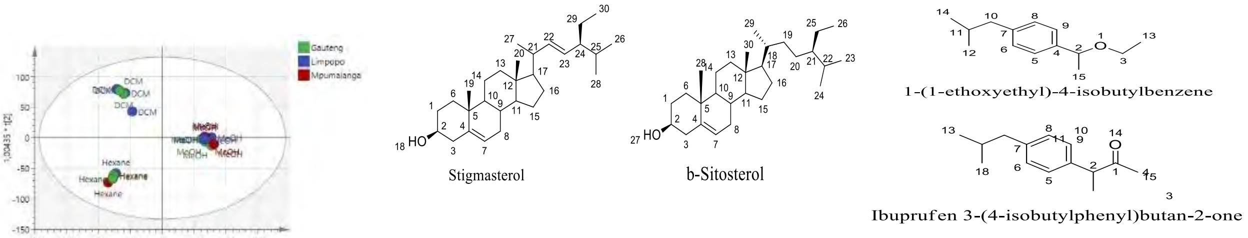
1D- and 2D-NMR Analysis

Structural elucidation

Fig 1: Flow chart diagram of obtaining pure compounds and isolation for UPLC-MS

Results and Discussion

Four compounds, ibuprofen (3-(4-isobutylphenyl) butan-2-one), 1-(1-ethoxyethyl)-4-isobutylbenzene, stigmasterol and β-sitosterol were isolated and identified by NMR spectroscopy. The UPLC-MS data revealed quantitative variations between samples sourced from different locations. The PCA scores plot revealed that chemical variations of *C. zeyheri* extracts were attributed to the extraction methods.



Stigmasterol

b-Sitosterol

1-(1-ethoxyethyl)-4-isobutylbenzene

Ibuprofen 3-(4-isobutylphenyl)butan-2-one

Fig 2: PCA scores plot derived from UPLC-MS data and structures of compounds isolated from *C. zeyheri*

Conclusions

Four compounds were isolated from the dichloromethane extract, and a chemometric plot revealed chemical variations attributed to different extraction methods and the geographical location of the plants.

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Investigating the use of metal-doped carbon dots as fluorescent probes for screening selected polycyclic aromatic hydrocarbons

Nomthandazo K. Ratsoma, *Sifiso A. Nsibande*

Department of Chemistry, Faculty of Natural and Agricultural Sciences, University of Pretoria, Lynnwood Road, Pretoria 0002, South Africa. E-mail: u16116870@tuks.co.za

Keywords: polycyclic aromatic hydrocarbon, carbon dot, fluorescence probe

Polycyclic aromatic hydrocarbons (PAHs) are persistent organic pollutants released into the environment through anthropogenic and natural activities [1]. Their carcinogenic, teratogenic, and mutagenic traits can have a negative impact on aquatic life and human health [2]. The lipophilic nature of PAHs and their typically low concentration levels in environmental water systems require highly sensitive detection methods for their continuous monitoring [3]. While chromatographic methods can offer excellent detection of these compounds, alternative screening methods can be cost-effective tools for large monitoring campaigns. Metal-doped carbon dots (M-CDs) are emerging as viable probes for sensitive detection of environmental pollutants, as they combine the inherent optical properties of CDs with the electronic properties of the metal centres [4].

In this study, therefore, fluorescent Zn-CDs and Fe-CDs were successfully prepared via a one-step hygrothermal process using citric acid as a carbon source and 1,2-phenylene-diamine as a nitrogen source. The morphological and optical properties of the obtained M-CDs were investigated using various techniques, including UV-vis, photoluminescence (PL), Fourier transform infrared (FTIR) spectroscopy, and transmission electron microscopy (TEM). The selected PAHs, namely phenanthrene and benzo[a]anthracene, were found to have a quenching effect (fluorescence “turn-off”) within 5 min upon their interaction with Zn-CDs and Fe-CDs within the 1.67×10^{-8} to 6.90×10^{-8} mol/L concentration range. The effect of the different doping metals on the sensitivity of CDs towards the detection of PAHs is reported. These preliminary results demonstrate the potential application of M-CDs for fluorescence screening of PAHs in environmental water samples at low concentrations.

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Comparison of passive and continuous flow extraction techniques for detecting IAS and NIAS migrating from plastic pollutants in surface water

Ross McAdam[a], *Madelien Wooding*[a] *and Elize Smit*[b]

[a]Department of Chemistry, University of Pretoria, Natural Sciences 1 Building, Hatfield, 0028, South Africa, E-mail: madelien.wooding@up.ac.za [b]Department of Chemical Sciences, University of Johannesburg, C2 Lab Building, Auckland Park, 2006, South Africa

Keywords: Extractables and Leachables, surface water, -sampling techniques, UPLC-HRMS

Ensuring good water quality is a key aspect of health in all communities; in the modern context this involves analysing our water sources. A major challenge to this is an ever-growing list of potentially harmful compounds which migrate into local water source. Plastics remain a substantial source of pollution in the environment, with global production exceeding 390 million tons. [1] Concerns have also risen regarding the potential leaching of residual intentionally added substances (IAS) and non-intentionally substances (NIAS) from these materials into water systems and potentially affecting human health.[2-5] Plastics in aquatic systems release both physical fragments and harmful chemicals. IAS and NIAS leach from plastics into surface waters, raising concern due to their toxicity, persistence, and lack of monitoring in Southern Africa.

This study compares two sampling methods for the detection of IAS and NIAS from surface waters collected at Rietvlei National Reserve. These methods compare a passive versus continuous flow extraction technique using a PDMS -sorbant material. 3D printed extraction devices were made for the continuous flow method. The extraction efficiency, detection limits, precision, and recovery of both methods were determined using targeted spiking experiments and analysed via UPLC with ion mobility coupled to high-resolution mass spectrometry (UPLC-IMS-HRMS). Preliminary screening results detected phthalate ester concentrations ranging from 1 ppb to 10 ppb in the samples.

Together, these complementary techniques address a critical sample preparation gap in trace-level plastic-associated contaminant detection. The project also contributes valuable occurrence data on polymer-derived contaminants in South African surface waters—supporting improved risk assessment and future mitigation strategies.

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Recovery of base metals and precious metals from spent RAM and CPU as secondary sources

Luthando Xolo[a], *Zenixole R. Tshentu*[a]

[a]Department of Chemistry, Nelson Mandela University, South Campus, Summerstrand, Gqeberha, 6001, South Africa, E-mail: s217070078@mandela.ac.za.

Keywords: Circuit boards, chelating ion exchangers, copper, nickel, platinum, palladium,

e-Waste has shown an exponential increase over the past 2 decades due to high demand for innovative technologies. This rise in e-waste is fueling the need to use advanced methods to recover precious and base metals found in the printed circuit boards. Chelating Ion exchangers have proved to be advantageous when compared with traditional methods of recycling printed circuit boards [1]. This is due to the high selectivity of the material which depends on metal ion of interest, concentration of metal ion and the functional groups of choice as donor atoms [2]. Ligands were synthesized with N and S donors to separate precious metals such as Pt, Pd, and Au from base metals and these were further separated using an anion exchanger for the separation of $PtCl_6^{2-}$, $PdCl_4^{2-}$ and $AuCl_4^-$, respectively. The Ligands were functionalized on Merrifield beads for base metals materials (Figure 1) and on silica for precious metals materials. These were characterized by FTIR, NMR, SEM and elemental analysis to confirm the successful synthesis and functionalization of the desired chelating ion exchangers. A solid/Liquid ratio was investigated, and the leaching solution of choice was optimized and was tested against aqua regia to check for the leaching efficiency. The different Chelating ion exchangers were used to obtain a precious metal rich solution and followed by a base metal rich effluent. The separation and recovery of these metals was achieved, and analysis was carried out using ICP-OES and X-Ray Diffraction to study the complexes obtained.

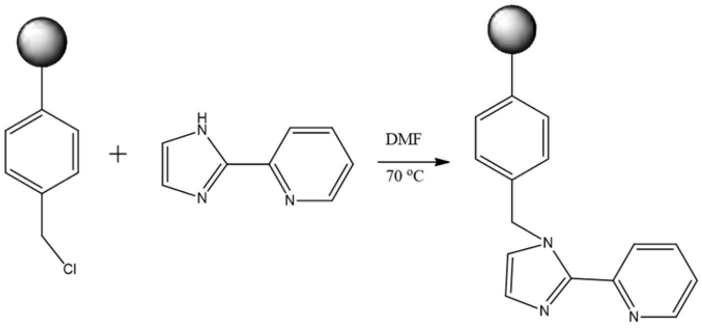

Figure 1. A schematic diagram for the synthesis of Merrifield beads functionalized with 2-(2-pyridyl)imidazole.

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Quantitative method development for the analysis of selected steroid hormones in WWTW influent and effluent: identification of seasonal trends

Celiwe Dlangalala, Xolani Nocanda and Brenda Moodley

Discipline of Chemistry, School of Agriculture and Science, University of KwaZulu-Natal, Westville Campus, Durban

Steroid hormones are endocrine disrupting compounds (EDCs) which are among the list of emerging contaminants identified by the United States Environmental Protection Agency (USEPA). The presence of these EDCs is hazardous to the environment and threatens the availability of clean, fresh water in rivers, dams, and lakes. They also compromise the quality of drinking water, leading to a loss of diversity due to their endocrine-disrupting capability, and food chain disruptions. For this reason, there is a need to develop analytical methods to analyse these endocrine-disrupting chemicals in wastewater, among other water bodies. In this work, the class of steroid hormones (estriol, bisphenol A, 17α-ethinylestradiol, levonorgestrel, medroxyprogesterone, progesterone, and mestranol) used in contraceptives was investigated due to their widespread use within the population of KwaZulu-Natal. This work aimed to determine the seasonal variations in concentrations between the dry and wet seasons for WWTW in the south, north, and outer west regions in Durban. Raw wastewater and effluent samples were collected at KwaMashu, Verulam, Isipingo, Kingsburgh, Hillcrest, and Hammarsdale WWTWs. An HPLC-UV-Vis method for determining steroid hormones was developed using a gradient system of methanol and water as the mobile phase. Extraction of the analytes was carried out using the solid phase extraction (SPE) method, which was optimised for solvent composition, SPE cartridge packing material, elution solvent volume, drying time, and pH. Optimum conditions were found using the HLB cartridges, drying for 30 minutes, and elution with 50% methanol /acetonitrile solvent composition using 10 mL solvent volume at neutral pH. The method was validated for recoveries which ranged between 97-112%, precision less than 15% RSD, LOD between 0.027-0.215 mg L^{-1}, and LOQ between 0.082-0.351 mg L^{-1}. The validated method was applied to samples collected during dry and wet seasons. Dry seasons gave higher concentrations compared to the wet season. Analyte concentrations in raw wastewater ranged between ND-0.73 mg L^{-1} during the wet season and 0.31-3.36 mg L^{-1} during the dry season. Effluent gave ND-0.010 mg L^{-1} during the wet season and ND-0.14 mg L^{-1} in the dry season. Precipitation was found to be the main factor during the wet season because increased rainfall diluted the steroid hormone concentrations. Results were statistically significant at a 95% confidence interval, meaning that steroid hormone concentration varies with seasons. The South region also recorded high concentrations of steroid hormones. This could be due to a high population density area, with the WWTW accepting mainly domestic waste.

Investigation of thermal separation probe (TSP) coupled to GC-MS for the analysis of long sulfur chains in complex matrices

Matodzi Tshiololi, Nolwazi Molefe, Boitumelo Motshabi and Nomandla Vela

Protechnik Laboratories, a Division of ARMSCOR SOC LTD, Centurion, 0157, South Africa, E-mail: matodzit@protechnik.co.za

Keywords: long sulfur chain, Thermal Separation Probe (TSP), *in situ* derivatisation, gas chromatography–mass spectrometry (GC-MS).

The analysis of long sulfur chain containing compounds is critical in environmental monitoring, chemical verification, and decontamination studies. However, challenges such as cross contamination, low recoveries, background interferences, volatility of analytes, and poor derivatisation of polar sulfur compounds hinder reliable analysis particularly in solid matrices like soil, clay, and leather.

This study investigates the application of the Thermal Separation Probe (TSP) coupled to a gas chromatography–mass spectrometry (GC-MS) for direct sample introduction and *in situ* derivatisation of long sulfur chains. TSP minimizes sample handling, reduces cross contamination, and enables efficient screening of polar and volatile analytes. The method was evaluated for recoveries in complex matrices, with best results obtained in soil at analyte concentrations above 20 µg/g.

Ethyl acetate, dichloromethane, and diethyl ether proved more effective than acetone in eluting these types of compounds from soil. *In situ* derivatisation was successful for multiple sulfur containing degradation products, although efficiency varied with thermal conditions and compound type.

Despite matrix specific limitations, TSP proved to be a robust, automated technique that enhances the effectiveness of GC-MS in identifying long sulfur chains. The method offers improved speed, sensitivity, and reliability for environmental and chemical safety applications.

The synthesis of 6-substituted chromone-2-carboxamide derivatives and their validation as corrosion inhibitors for selected metals in acidic medium

S.S. Nyembe, I.D.I. Ramaite, M.M. Kabanda, L.C. Murulana

Department of Chemistry, Faculty of Science, Engineering and Agriculture, University of Venda, Thohoyandou, 0950,
E-mail: Siyabonga.Sihle@univen.ac.za

Keywords: gradual deterioration, gravimetric analysis, inhibition efficiency, Langmuir adsorption, adsorption films

Corrosion refers to the progressive degradation of a metal’s properties resulting from its interaction with the surrounding environment. Although corrosion is unavoidable, it must be effectively controlled to ensure that equipment continues to function efficiently and reliably. One approach to corrosion control is prevention through corrosion inhibition, where small quantities of specific chemical compounds known as inhibitors are introduced into a corrosive medium to reduce the rate of metal deterioration [1–4].

In this study, a series of non-toxic, cost-effective 6-substitutedchromone-2-carboxamide derivatives (Chr-2-Carb, Br-Chr-2-Carb, Cl-Chr-2-Carb, CH_3O-Chr-2-Carb, and NO_2-Chr-2-Carb) were synthesized and tested for their corrosion inhibition performance on mild steel (MS), zinc (Zn), and aluminium (Al) in acidic media—specifically, 1.5 M HCl for MS and Zn, and 1.0 M HCl for Al. Both experimental and computational techniques were employed, including nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry, Fourier-transform infrared (FTIR) spectroscopy, gravimetric analysis (GA), electrochemical measurements, density functional theory (DFT) calculations, and surface morphology characterization. Gravimetric results for MS demonstrated that inhibition efficiency (%IE) increased with inhibitor concentration, with NO_2-Chr-2-Carb achieving the highest %IE (97.44%). Adsorption data conformed to the Langmuir isotherm model for all compounds across the tested metals. All synthesized inhibitors effectively reduced corrosion rates, exhibiting mixed-type inhibition for Al and MS, and predominantly physical adsorption for Zn.

FTIR results confirmed the formation of adsorbed protective films on the metal surfaces. Potentiodynamic polarization (PDP) indicated that these inhibitors slowed both anodic and cathodic corrosion processes, consistent with Tafel polarization findings. Electrochemical impedance spectroscopy (EIS) revealed larger imperfect semicircle diameters with increasing inhibitor concentration, corresponding to higher surface coverage and increased charge transfer resistance. SEM/EDS and contact angle measurements confirmed that the inhibitors generated hydrophobic protective layers, effectively blocking corrosion sites. Quantum chemical calculations further elucidated the strong interactions between inhibitor molecules and the metal surfaces, supporting the experimental findings.

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Synthesis and characterization of natural deep eutectic acid ferrofluids and their application for fluoroquinolone determination in food samples.

Mulusew B. Yizengaw, *TA Makwakwa, D. Moema and V Pakade*

Department of Chemistry, College of Science, Engineering and Technology (CSET), University of South Africa, Florida Science Campus, 1709, Johannesburg, South Africa

Keywords: Deep eutectic solvent, ferrofluid, antibiotics, magnetic nanoparticles, green chemistry

Ferrofluids are colloidal systems that consist of a single domain of magnetic nanoparticles dispersed in a liquid carrier [1]. Their use in liquid-phase microextraction techniques has become increasingly popular due to several advantages, including ease of operation, rapid extraction, and reduced use of organic solvents [2]. This study proposes a green and efficient extraction technique that utilizes ferrofluids, which are based on magnetic nanoparticles combined with a hydrophobic deep eutectic solvent for the pre-concentration and determination of fluoroquinolones in food samples, followed by analysis using high-performance liquid chromatography (HPLC). The magnetic nanoparticles were synthesized using an environmentally friendly method that incorporates an extract from the Hibiscus rosa-sinensis flower, which serves as both a reducing and stabilizing agent. The extract contains various chemical compounds, such as organic acids, phenolic acids, and flavonoids, which are essential for the reduction and stabilization of metal nanoparticles. This approach aims to generate safer and more environmentally friendly functional materials, in line with sustainable nanomaterial synthesis principles. Analytical techniques, including scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX), were employed to investigate the surface morphology and elemental composition of the magnetic nanoparticles. Preliminary results from SEM imaging show variations in particle size and aggregation patterns. Additionally, the EDX spectrum confirmed the presence of iron (Fe), carbon (C), and oxygen (O) elements in the nanocomposite.

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Landfill leachates characterisation and the application of magnetic iron oxide nanoparticles for adsorptive removal of toxic elements

Mpho Mautla, Alseno K. Mosai and Patrick G. Ndungu

Department of Chemistry, University of Pretoria, Lynwood Road, Pretoria, 0002, South Africa, E-mail: u18175474@tuks.co.za.

Keywords: iron oxide nanoparticles, adsorption, heavy metals, landfill, leachates

Landfill leachates contain toxic pollutants, which often leach out to the environment. There is therefore a need for innovative wastewater and leachate remediation techniques that can remove a range of toxic pollutants[1]. This study has sampled raw landfill leachates generated by landfilled municipal solid waste (MSW) and industrial waste from Gauteng province, South Africa. The study aimed to characterise the leachates by determining their physicochemical parameters and by identifying and quantifying the elements in the leachates using advanced spectroscopic analytical techniques. Furthermore, the study aimed to investigate the efficiency of the removal of toxic elements from the landfill leachates using synthesised iron oxide nanoparticles[2]. Magnetic iron oxide (Fe_3O_4) nanoparticles were synthesised through a co-precipitation method using the precursors $FeCl_3 \cdot 6H_2O$ and $FeCl_2 \cdot 4H_2O$[3]. X-ray diffractometer (XRD) instrument, Transmission Electron Microscopy (TEM), Scanning Electron Microscopy combined with Energy dispersive X-ray spectroscopy (SEM/EDX), X-ray photoelectron spectroscopy (XPS), and Fourier transform infrared spectroscopy (FTIR) were used to characterise the nanoparticles. A comparison of the composition of the MSW and industrial waste landfill leachates was performed. The results indicated that the industrial leachate had high concentrations of toxic elements, including Cd, Cr, As and Pb. These elements were also detected in the MSW leachate but in low concentrations. Overall, the concentrations of toxic elements in leachates were alarming, indicating the urgent need for their removal from both industrial and MSW landfill leachates. The magnetic iron oxide nanoparticles will be tested as a potential adsorbent for both leachates.

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Development of biodegradable edible film based on aloe ferox and ZnO nanoparticles for postharvest packaging

Jerry O. Adeyemi[a,b]*, and *Olaniyi A. Fawole*[a,b]

[a] Postharvest and Agroprocessing Research Centre, Department of Botany and Plant Biotechnology, University of Johannesburg, P.O. Box 524, Auckland Park, Johannesburg 2006, South Africa. [b] South African Research Chairs Initiative in Sustainable Preservation and Agroprocessing Research, Department of Botany and Plant Biotechnology, University of Johannesburg, Johannesburg 2006, South Africa. jerryadeyemi1st@gmail.com

Keywords: Edible film, Rooibos spent waste, ZnO nanoparticles, Aloe ferox, Active packaging.

Food security remains a pressing global issue, exacerbated by rapid population growth, rising food demand, postharvest losses, and microbial contamination, all which compromise food availability and safety [1]. Innovative food packaging offers a promising solution with capacity to extend shelf life, especially upon functionalization with material such as nanoparticles, reducing spoilage, and preserving food quality during storage and transportation [1]. Aloe ferox (Cape Aloe), a hardy medicinal plant native to South Africa, has emerged as a suitable biopolymer candidate due to its polysaccharide-rich composition, biocompatibility, and antioxidant properties. In this study, spent rooibos leaves, an agro-waste byproduct, were utilized as a sustainable resource for synthesizing zinc oxide nanoparticles (ZnO NPs), promoting a circular bioeconomy. The ZnO NPs were incorporated into an Aloe ferox-based biopolymer matrix at varying concentrations to develop an edible film for food packaging. The physicochemical properties of the ZnO NPs and AFM/CNF/ZnO-NPs composite films were analyzed using Fourier Transform Infrared Spectroscopy (FTIR), Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), and Energy Dispersive X-ray Spectroscopy (EDX), alongside mechanical and barrier property evaluations. Biological assessments revealed a dose-dependent antioxidant response and antimicrobial activity against foodborne pathogens for the composite material. Additionally, the incorporation of ZnO NPs enhanced the mechanical and barrier properties of the films, making them effective than the control. Overall, these findings highlight the potential of Aloe ferox-ZnO NP films as sustainable active packaging materials, aligning with the United Nations Sustainable Development Goals (SDGs) on sustainability, eco-friendliness, waste valorization, and food security. The study underscores the importance of green nanotechnology in developing next-generation food packaging solutions with antimicrobial functionality and improved physicochemical properties.

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Reduced graphene oxide ion imprinted polymer rGO nanocomposite-Sensor tackling cadmium pollution

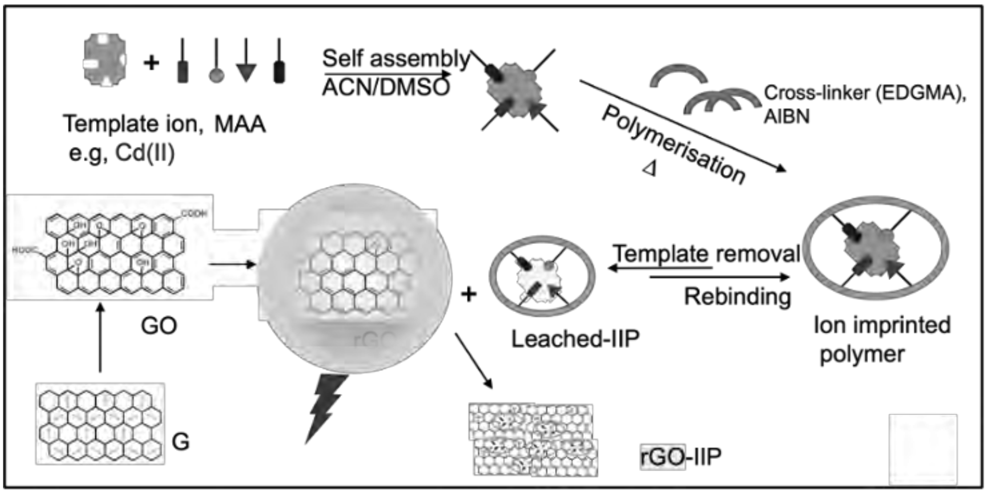
Sifelani Dube, *Abayneh A. Ambushe and Messai A. Mamo*

Department of Chemical Sciences, University of Johannesburg, South Africa, E-mail: sifelanid@uj.ac.za.

Keywords: cadmium, chemiresistor, nanocomposite, graphene

Cadmium (Cd) contamination in water remains a critical environmental and public health challenge due to its high toxicity and persistence. Conventional analytical techniques, while accurate, are costly, laboratory-bound, and unsuitable for real-time field monitoring [1]. This work reports the development of a portable chemiresistive sensor integrating electrochemically reduced graphene oxide (rGO) with an ion-imprinted polymer (IIP) for detection of ultra-trace level Cd(II) in water. The optimized 1:3 IIP:rGO nanocomposite, drop-cast onto interdigitated gold electrodes, exhibited rapid response times (<60 s), excellent reproducibility (%RSD < 2.1%), and long-term stability (<10% drift over 90 days). The sensor demonstrated high selectivity against competing ions and achieved a low detection limit of 0.704 μgL^{-1}, below the WHO and SANS drinking water guideline (3 μgL^{-1}). Percentage recovery studies by spiking Cd(II) in borehole and river water confirmed the accuracy of the method and its applicability for environmental monitoring (95.9–103%) [2]. These findings highlight the potential of rGO–IIP chemiresistive sensors as cost-effective, scalable tools for on-site water quality assessment, advancing sustainable pollution management and public health protection.

Structure Block/Scheme.



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Where are we now on environmental forensics?

Christina Kannigadu[a], Alexander Whaley[a]

[a]*LECO Africa, Gauteng, 1619, South Africa, E-mail: Christina@lecoafrica.co.za*

Keywords: GC×GC-TOFMS, Non-target Screening, POPs, PAHs, PCBs, Pollutant fingerprinting

Environmental forensics has progressed from basic chemical analysis to advanced multi-dimensional chromatographic techniques, driven by the increasing complexity of environmental crimes. Early investigations relied primarily on single-dimensional gas chromatography coupled with mass spectrometry (GC-MS) to detect pollutants such as dioxins, polychlorinated biphenyls (PCBs), and polycyclic aromatic hydrocarbons (PAHs). However, cases such as the Mandara dioxin investigation and the analysis of incinerator residues—which contained pyrolysis-resistant compounds including polychlorinated dibenzodioxins (PCDDs), polychlorinated dibenzofurans (PCDFs), PCBs, PAHs, and other chlorinated aromatics—highlighted the limitations of these traditional methods.

The crocodile mortality in the Olifants River, linked to pansteatitis and associated with multiple low-level contaminants including organochlorine pesticides, furans, and heavy metals, further demonstrated the need for more sensitive and comprehensive analytical approaches.

Modern environmental forensics increasingly employs Time-of-Flight Mass Spectrometry (GC-TOFMS) and Comprehensive Two-Dimensional Gas Chromatography–TOFMS (GC×GC-TOFMS). These techniques provide superior separation of co-eluting compounds, non-targeted screening of complex environmental samples, and improved pollutant source attribution. Sample preparation has also advanced, with tools such as Twister® enabling efficient extraction of trace-level pollutants from water, sediments, and biological tissues.

As environmental crimes become more sophisticated, these advanced tools provide investigators with the ability to reconstruct contamination events, identify responsible parties, and strengthen environmental crime prosecution.

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Development and validation of cost-effective HPLC methods for the quantification of major chemical constituents of *Sutherlandia frutescens*

Michaela Mouton[a], *Edith M. Antunes*[b] *and. Denzil R. Beukes*[a]

[a] School of Pharmacy and [b] Department of Chemistry, University of the Western Cape, Robert Sobukwe Road, Bellville 7535, South Africa, E-mail: 4426276@myuwc.ac.za

Keywords: *Sutherlandia frutescens*, HPLC, Method validation, Phytochemical analysis

Sutherlandia frutescens (Cancerbush) is a widely used South African medicinal plant with a longstanding history in South Africa as a traditional medicine. Its therapeutic properties have been attributed, in part, to two major classes of phytochemicals: the flavonoid glycosides sutherlandins A-D and cycloartane-type triterpene glycosides sutherlandiosides A-D, which serve as chemotaxonomic markers. Despite the plant's popularity and medicinal potential few studies have reported validated methods for quantifying these phytochemicals. This is an essential step for quality control and the preparation of well-characterized extracts for biological studies.

This study reports the development and validation of a robust and affordable HPLC-UV method for the quantification of sutherlandins A-D and preliminary method development for the triterpene glycosides sutherlandiosides A–D in both commercial formulations and plant samples.

Separation of the sutherlandins were achieved using a Zorbax Eclipse XDB-C18 column with an acetonitrile–formic acid gradient and UV detection at 370 nm. The method yielded baseline separation within 20 min, with excellent linearity ($R^2 > 0.9995$), precision (RSD < 3%), recovery (95–105%), and LOQs of 5.5–8.1 µg/mL.

In addition, we demonstrate UV-based detection of sutherlandiosides at 210 nm, eliminating the need for more expensive ELSD or LC-MS-based methods. Using a Hydro-RP column under isocratic elution in 12 min, preliminary results are promising and full validation is ongoing.

Together, these methods offer a practical, scalable platform for routine quality control, standardization, and research into *S. frutescens* phytochemistry in resource-constrained settings.

Method validation for the determination of volatile organic compounds in environmental samples using GC-FID

Masejeng Leso, Boitumelo Motshabi and Nomandla Vela

Protechnik Laboratories, a Division of ARMSCOR SOC LTD, Centurion, 0157, South Africa, E-mail: masejengl@protechnik.co.za.

Keywords: VOCs, gas chromatography (GC), flame ionisation detector (FID), limit of detection (LOD)

Volatile organic compound (VOC) analysis is important for the assessment of environmental pollution, monitoring of air quality, as well as ensuring compliance with health and safety regulations, due to the potential toxicity of VOCs and impact on human health. This study presents the validation of a gas chromatography-flame ionisation detector (GC-FID) method for the analysis of selected volatile organic compounds (VOCs) in environmental samples. The method was optimized by attaching a Headspace autosampler to eliminate sample preparation and achieve high recovery.

The validation process assessed key performance parameters, including selectivity, precision, accuracy, linearity and detection limits. A calibration curve was constructed using spiked water and air samples, yielding a coefficient of determination (R2 > 0.98) demonstrating good linearity across the working concentration range. Accuracy was evaluated through spike-recovery experiments, with recoveries ranging between 94 % and 120 %, confirming method reliability. Precision, assessed as repeatability and reproducibility, showed relative standard deviations (RSDs) below 10 %. The method limit of detection (LOD) and limit of quantification (LOQ) were determined to be in the low parts-per-million (ppm) range, covering the working range.

The validated method provides a reliable and robust tool for the routine analysis of VOCs in environmental samples, providing critical support for quality assurance and environmental safety practices.

MOF-derived high-entropy spinel oxide(($(CoCuFeMnNi)_3O_4$) as bifunctional electrocatalysts for rechargeable zinc-air batteries

Helen A. Chernet, *Aderemi B. Haruna, Augustus K. Lebechi, and Kenneth I. Ozoemena*

Molecular Science Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Johannesburg, 2050, South Africa, E-mail: 2787681@students.wits.ac.za.

Keywords: Metal organic framework, High entropy spinel oxide, Oxygen reduction reaction, Oxygen evolution reaction, Zinc air battery

In recent years, the rapid growth of renewable energy applications has driven a significant demand for efficient large-scale energy storage solutions. Among various options, rechargeable zinc-air batteries (RZABs) have emerged as a promising technology due to their high energy density, sustainability, and cost-effectiveness.[1] Consequently, attention has been focused on improving the air electrode for high performance RZABs, highlighting the urgent need to develop electrocatalysts with abundant active sites and long-term stability.[1,2] High entropy spinel oxide (HESOx) offers a promising platform by incorporating multiple metal cations into the crystal lattice, enabling entropy stabilization, lattice distortion, and enhanced chemical and thermal stability.[3] In this study, MOF-derived high entropy spinel oxide $(CoCuFeMnNi)_3O_4$ electrocatalyst materials were synthesized via both microwave-assisted and solvothermal methods to evaluate their bifunctional catalytic activities toward oxygen evolution (OER) and oxygen reduction reactions (ORR). The choice of MOF-derived synthesis is based on the well-defined architecture and atomic-level dispersion of metal centers in MOFs, which enables precise control over the morphology and uniform distribution of metal species in the resulting multi-metal oxides. XRD analysis confirmed the formation of spinel oxide phase, and thermogravimetric analysis (TGA) showed high thermal stability. The materials were further characterized by SEM, HRTEM, FTIR, Raman, XPS and BET surface area analysis. Electrochemical measurements demonstrated notable bifunctional activities. For ORR, the microwave synthesized sample exhibited a half wave potential ($E_{1/2}$) of 0.88 V vs. RHE and a Tafel slope of 69 $mVdec^{-1}$, compared with 0.86 V and 71 $mVdec^{-1}$ respectively for solvothermal sample. While for OER, the overpotential at 10 $mAcm^{-2}$ were 410 mV and 390 mV for microwave and solvothermal electrode materials, respectively. These results demonstrate the influence of synthesis methods on the electrocatalytic behaviors of high entropy spinel oxides and support their potential as efficient bifunctional catalysts for RZABs applications.

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Bio-inspired calcium-doped manganese oxide via microwave synthesis as a bifunctional oxygen reduction and evolution electrocatalyst

Ernst Hechter[a], *Dean Barrett*[a] *and Kenneth Ozoemena*[a]

[a]*School of Chemistry | University of the Witwatersrand | Private Bag 3 | PO WITS 2050 | South Africa. E-mail: 1890762@students.wits.ac.za*

Keywords: biomimicry, electrocatalysis, manganese oxides, OER, ORR, RZAB

The oxygen evolution and oxygen reduction reactions (OER and ORR, respectively) are of critical importance, both to science and industry and to most living systems. The OER is the energy-hungry oxidation of water or hydroxide to yield elemental dioxygen, and is a limiting reaction in water splitting and rechargeable metal-air batteries. The ORR is the reverse reaction, the reduction of elemental oxygen to yield energy and water or hydroxide. It is therefore critical in fuel cells and metal-air batteries. This has made ORR and OER catalysis a thriving research area for decades, in both biological and inorganic systems. Despite tens of thousands of publications in the last ten years alone,[1] efficient and cost effective catalysts remain elusive.

Calcium, manganese and oxygen form the active sites of photosystem 2, a natural OER catalyst. Calcium doping or calcium based materials have given high OER/ORR activities, high oxygen defect concentrations and allow mechanisms involving p-band electrons as opposed to d-band only materials.[2–4] Computational studies have shown that calcium doping of manganese oxides allows water oxidation to follow lower energy pathways.[5] Calcium-manganese post-spinel oxide has itself also shown promise as an ORR catalyst.[6]

In this work, Hausmannite phase manganese oxide was doped with calcium to form metal oxide on onion-like carbon composites. These were synthesized using hydrothermal and microwave methods. The incorporation of calcium yielded significant improvement to the OER, while ORR was unchanged. The microwave syntheses, in addition to being 11 hours quicker than the hydrothermal method, also gave composites with superior electrochemical performance.

The improved performance was analysed using XPS, XRD and microscopy in addition to thorough 3-electrode testing, and performance analysis in a real zinc-air battery. These methods allow a tentative description of a Ca-Mn active site, which is compared to the Ca-Mn site of photosystem II. Overall, this works presents a simple, low cost method to produce biomimetic catalysts for oxygen evolution, as well as adding to the growing body of evidence that microwave synthesis can enhance the properties of products, even when the same phase is produced.

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A new electrochemical sensor based on magnetic nanoparticles-molecularly imprinted polymer for trimethoprim detection

Hopewell Mnyandu[a], *Precious Mahlambi*[a], *and Mun'delanji Vestergaard*[b]

[a] Department of Chemistry, University of KwaZulu-Natal, Private Bag X01, Scottsville, Pietermaritzburg,3209, South Africa, E-mail: 212539071@stu.ukzn.ac.za. [b] Faculty of Agriculture, Kagoshima University, Kagoshima City 890-0065, Japan.

Keywords: molecularly imprinted polymers, electrochemical, polymerization, glassy carbon electrode, magnetic nanoparticles, trimethoprim

This work presents the development of a novel electrochemical sensor for the selective detection of trimethoprim, an antibiotic, using molecularly imprinted polymers (MIPs). The electrochemical sensor development involved the polymerization of methacrylic acid as the functional monomer and ethylene glycol methacrylate as the cross-linker, initiated by 1,1′-azobis(cyclohexanecarbonitrile), in the presence of trimethoprim as the template molecule. Magnetic iron oxide nanoparticles were incorporated to enhance electrochemical sensor performance. The MIP was drop-casted on a glassy carbon electrode serving as the transducer, with phosphate buffer saline employed as the electrolyte. Electrochemical characterization of the modified electrode was conducted using cyclic voltammetry within a potential window of −1.0 to +1.0 V. Analytical detection of trimethoprim in real water samples was achieved through differential pulse voltammetry and electrochemical impedance spectroscopy, demonstrating high sensitivity and selectivity. This work highlights the potential of MIP-based electrochemical sensors integrated with magnetic nanoparticles for environmental monitoring of antibiotic contaminants.

An investigation into electrochemical and physicochemical properties of cathode oxide-based material used in Sodium-Ion Batteries

Yibanathi Mlozana, Ernst Ferg, Xandri van Niekerk, and Funmilola Adesanya

Department of Chemistry and uYilo e-Mobility Programme, Nelson Mandela University, PO Box 77000, Port Elizabeth, 6031, South Africa, E-mail: s224365223@Mandela.ac.za, Ernst.Ferg@mandela.ac.za

Keywords: Sodium-ion batteries, Electrochemical, Physicochemical, Layered Metal Oxides

Sodium-ion Batteries (SIBs) are being used as an alternative to Lithium-ion batteries (LIBs) due to several demonstrated advantages, including safety, capacity, cycling stability, lower manufacturing costs, and a larger abundance of sodium when compared to lithium. Additionally, SIBs are posited to exhibit similar physicochemical and electrochemical properties to LIBs under room temperature conditions, enabling their use in large-scale applications, such as energy storage for electrical grid development. Although the energy storage industry appears to be progressing well with the discoveries surrounding cathode materials used in SIBs, understanding the chemistry involved in their synthesis, as well as the electrochemical mechanism, remains worthwhile to investigate. Approximately 60% of the cost of battery manufacturing is attributed to the synthesis and manufacturing of the cathode (positive electrode); hence, understanding the chemical phase transitions during its synthesis route can serve as a crucial step in the overall battery manufacturing process and related analysis. Currently, the SIBs market is primarily centred on three broad categories of cathode active materials, including Prussian Blue and its analogues, NASICON types, and Layered Metal Oxides (LMOs). This project aims to study the thermal synthesis route of the LMO for cathode materials typically used in Na-ion batteries, to investigate the electrochemical and physicochemical changes that occur, leading to the final stable electroactive phase transition.

For this project, layered metal oxides ($NaM_xMn_{1-x}O_2$) were synthesised and doped with M = Mg, Al, Ag, Cu, Ni, Fe, Ni-Fe, and Co, respectively, where x ranged between 0.05 – 0.5. In each case, precursors were dissolved in water and citric acid. Results by using Powder X-ray Diffraction (PXRD) analysis showed that all doped precursors consisted of highly crystalline multiphase materials that, upon heating, their respective structures collapsed predominantly, forming amorphous intermediates between 300 °C and 400 °C. Further heating up to 900 °C led to the formation of the desired crystalline orthorhombic type of structure (Figure 1). In this study, the focus will be on elucidating the cobalt-doped layered structure.

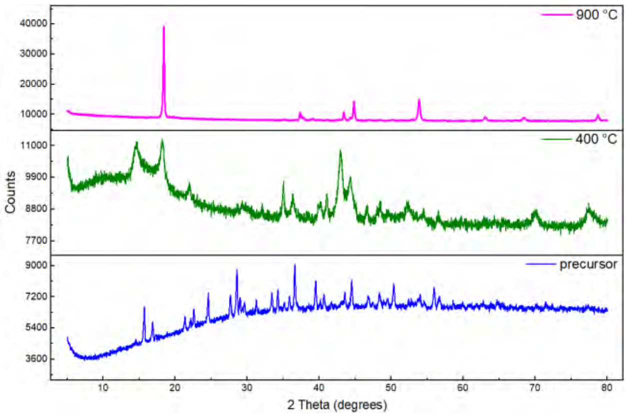

Figure 1: PXRD diffraction patterns obtained using a Panalytical Aeris diffractometer with Co radiation. The progression of the phase transitions by heating to different temperatures of the cobalt-doped LMO $Na_{0.67}Co_{0.5}Mn_{0.5}O_2$ are shown.

High-entropy spinel oxide $(CoCuFeNiMn)_3O_4$ as bifunctional electrocatalyst for rechargeable zinc-air battery

Nkgaetsi M. Ngoepe[a], *Thapelo P. Mofokeng*[a], *Aderemi B Haruna*[a], *and Kenneth I. Ozoemena*[a]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Johannesburg 2050, South Africa, e-mail: 2235779@students.wits.ac.za.

Keywords: High-entropy spinel oxide, oxygen evolution reaction, rechargeable zinc-air battery

A superior non-noble air-cathode electrode material is a long-term goal for the next generation of rechargeable zinc-air battery (RZAB) applications due to its safety, low cost, and environmental friendliness compared to Lithium-ion batteries [1, 2, 3]. In this work, efficient high-entropy spinel oxide $(CoCuFeNiMn)_3O_4$ cathode material for oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) were prepared by laminar flow-assisted co-precipitation and annealed at different temperatures (500, 750, and 900 ºC). The materials were abbreviated $HESOx_L$-500, $HESOx_L$-750, and $HESOx_L$-900. The physical properties of the materials were analysed with X-ray diffraction (XRD), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). XRD confirmed the formation of spinel oxide structure shown by 311 miller indices, SEM showed the effect of different annealing temperatures forming different particle sizes, and XPS showed the presence of different metals and their oxidation states. The bifunctionality of the materials were studied using electrochemical measurement in a three-electrode system, for ORR the half-wave potential ($E_{1/2}$) followed the order $HESOx_L$-900 < $HESOx_L$-500 < $HESOx_L$-750, while for OER at 10 mA/cm^{-2} current density $HESOx_L$-500 was the highest at 1.60 V (($HESOx_L$-750 (1.63 V) and $HESOx_L$-900 (1.64 V)). This good OER performance of $HESOx_L$-500 is governed by partially filled valence band that allows faster formation of $^*OOH$. The application was extended to an in-house three-dimensional rechargeable zinc-air battery cell. $HESOx_L$-500 showed good stability with long cycling of 200 hours, discharge areal energy of 44.4 $mWh/cm^2_{geometric}$ and power of 101.6 mW/cm^2. Discharge areal energy obtained outperform the benchmark of 35 $mWh/cm^2_{geometric,}$ which relate to specific energy of Li-ion 120 Wh kg_{pack}. This work highlights a rational design of cathode material, a low-cost and application in a robust RZAB.

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Influence of doping and synthetic parameters on LAMOX for advanced solid oxide fuel cells

Zukiswa C. Mbande[a], *Caren Billing*[a] *and Dave G. Billing*[a]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, 2001, South Africa, E-mail: 0603854F@students.wits.ac.za.

Keywords: LAMOX, EIS, XRD, dopants

Solid oxide fuel cells (SOFCs) is an emerging technology utilized to address the lack in sustainability of energy generation. Solid oxide electrolytes are generally operated between 800 – 1000 ℃, which is energy intensive for starting up and leads to material degradation. Thus the development of alternative electrolytes with enhanced ionic conductivities capable of operation at intermediate temperatures (400 – 600 ℃) is essential. In this vein, materials such as LAMOX ($La_2Mo_2O_9$) are being investigated as solid electrolytes and have demonstrated higher ionic conductivities than the commercially used yttria stabilized zirconia (YSZ) electrolyte at these intermediate temperatures.

LAMOX exists in two distinct temperature dependent crystallographic phases, namely, monoclinic α (< ± 580 ℃) and cubic β (> ± 580 ℃). The figure shows a distinctive powder X-ray diffraction (PXRD) peak which exhibits the $La_2Mo_2O_9$ α to β transition at ~580 °C. The β-$La_2Mo_2O_9$ is the desired phase as its ionic conductivity is two orders of magnitude higher than that of α-$La_2Mo_2O_9$ [1]. Stabilization of the β-$La_2Mo_2O_9$ to room temperature is thus vital. This has been achieved through doping with cations such as Y^{3+}, Dy^{3+} and Nd^{3+} at the La^{3+} site, and V^{5+}, W^{6+} and Cr^{6+} at the Mo^{6+} site [2]. Research has focused mainly on double doping to stabilise the β-$La_2Mo_2O_9$ phase and offer the potential to increase the conductivity. We therefore propose a systematic approach to develop a Y^{3+} and W^{6+} co-doped LAMOX system, using the sol-gel synthesis method. Rietveld refinement of PXRD data, including synchrotron data, showed that doping with Y^{3+} ($La_{2-x}Y_xMo_2O_9$; $0.1 \leq x \leq 0.4$) stabilizes the β-phase. Also evident was a decrease in the thermal expansion co-efficient with an increase in Y^{3+} content. These initial findings highlight the potential of Y^{3+} doped $La_2Mo_2O_9$ system and thus the Y^{3+}-W^{6+} co-doped system will be further investigated as an intermediate temperature SOFC electrolyte.

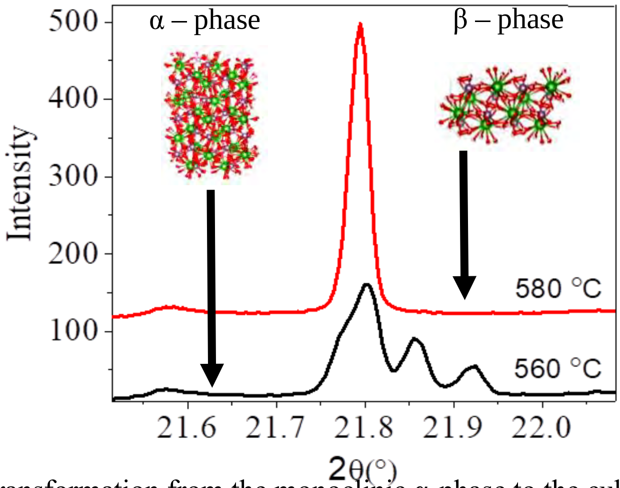

Figure 1: The phase transformation from the monoclinic α-phase to the cubic β-phase (inset) is clearly illustrated by the change in peak profile of the (321) reflection.

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Manganese oxide-based electrochemical sensor for the detection of dopamine

Lebohang Morake, Dhielnawaaz Abrahams and Priscilla G. Baker

SensorLab research group, Chemistry Department, University of the Western Cape, Robert Sobukwe Road, Private Bag X17, Bellville, 7535
E-mail: 4496130@myuwc.ac.za, dhabrahams@uwc.ac.za, pbaker@uwc.ac.za

Keywords: Manganese oxide, Electrochemical sensors, Dopamine sensing

Dopamine (DA; 3,4-dihydroxyphenethylamine) is a neurotransmitter [1], involved in regulating various systems including the central nervous system, endocrine functions and cardiovascular system [2,3]. DA governs cognitive and neuroendocrine functions, emotions and sleep [4]. Typically, DA concentrations in brain fluids lie in the range 10^{-6} - 10^{-8} M [5] and deviations from this normal range are associated with susceptibility to disorders such as Schizophrenia, Parkinson's and Huntington's disease [6,7] as well as other central nervous system conditions including depression and anxiety [8]. Monitoring DA is therefore essential because sensing platforms capable of detecting DA at physiological levels could play an important role in early prevention and clinical diagnosis of the aforementioned diseases.

In this work we report the fabrication of a manganese oxide-based electrochemical sensor for sensitive determination of dopamine in model aqueous solutions (0.1 M phosphate-buffered saline (PBS), pH 7.3). Manganese oxide thin films were prepared on glassy carbon electrodes via chronoamperometry; we explored deposition times of 30, 60, 120, 240 and 600 seconds to optimize film formation, with the aim of forming a high surface area modified electrode.

The as-synthesized thin films were characterized by scanning electron microscopy (SEM), energy dispersive x-ray spectroscopy (EDX) and atomic force microscopy (AFM) and electrochemical techniques.

Post-synthesis and characterization, dopamine sensing by cyclic voltammetry (CV) and square wave voltammetry (SWV) was carried out with E600s. The modified electrode exhibited a limit of detection (LOD) of 3.95 ± 0.03 µM (n=3) which lies within physiological DA concentrations; the linear response was observed over 1.67-16.4 µM. Complementary UV-Visible absorbance measurements showed a 2.93% decrease in DA absorbance before and after SWV oxidation while also indicating that 97.1% of DA remains in the bulk solution.

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Sodium-potassium dual pre-intercalated alpha manganese dioxide cathode material for high-performance aqueous zinc-ion batteries

T.P Mofokeng, *A.B Haruna*, *K.I Ozoemena*

Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, PO Wits, Johannesburg 2050, South Africa

Keywords: Dual doping, Couette-Taylor flow reactor, pre-intercalation, zinc-ion batteries

Manganese dioxide is a promising cathode material for aqueous zinc ion batteries (AZIBs) due to its high theoretical capacity, _operating voltage, abundance and low cost.[1] However, the dissolution of MnO_2 and the disproportionation of Mn^{3+} result in irreversible reactions and significant structural degradation during prolonged charge/discharge cycles, which limits their commercial viability. In addition, there are still some challenges in fabricating cathode materials that can deliver excellent performance, while also being simple and less costly to produce in large quantities. In this study, we have utilized a two-step synthetic method: Couette-Taylor flow reactor and hydrothermal method to produce alpha manganese oxide pre-intercalated with sodium and potassium ions. The pre-intercalation of Na^+ and K^+ stabilizes the tunnel structure and has the effect of electrostatic shielding to facilitate the (de)intercalation of $Zn2^+$.[2] X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and transmission electron microscopy (TEM-ESD) coupled with energy dispersive spectroscopy analyses confirm the successful synthesis of $Na^+/K^+@\alpha\text{-}MnO_2$. The $Na^+/K^+@\alpha\text{-}MnO_2$ cathode showed a specific capacity of 310 mAh g^{-1} when subjected to a current density of 0.1 Ag^{-1}. This capacity exceeds that of the same cathode material synthesised through a conventional method (253 mAh g^{-1}) under the same current density conditions. The enhanced electrochemical performance is attributed to the flower-like morphology and the synergistic effect of dual metal ion pre-intercalation, which created open active sites and conductive structures, facilitating the diffusion of hydrogen and zinc ions and improving the overall capacity of the cathode material.

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Methods of improving the performance of semiconductors in the photoelectrocatalytic degradation of organic pollutants in wastewater

Omotayo Arotiba, Dimpo S. Sipuka, Tsholofelo I. Sebokolodi, Kehinde D. Jayeola, Gugulethu P. Ndima, Oluchi V. Nkwachukwu*

[a] *Department of Chemical Sciences, University of Johannesburg, Doornfontein, 2028, South Africa*
[b] *Centre for Nanomaterials Science Research, University of Johannesburg, South Africa*

Keywords: Photoelectrocatalysis; semiconductor; doping; morphology control; heterojunction; water treatment

Photoelectrocatalysis (PEC), a subset of electrochemical advanced oxidation processes, can be a complementary and sustainable water treatment technology to the existing water treatments methods. This method can also be engineered towards decentralized wastewater treatment technology for the treatment of industrial wastewater for water re-use. The overall performance of a PEC system depends on the efficiency of the photoelectrode (photoanode and photocathode) in terms of light absorption, charge generation and charge separation among other factors [1]. Thus, an important aspect of research in PEC is to develop new or improved materials and photoelectrodes. While the preparation of novel materials is interesting, other approaches include the engineering of existing semiconductors in the fabrication of photoelectrodes towards improved PEC performance. This paper highlights how we engineer semiconductors using doping [2], morphology control [3] and heterojunction formation [4] to improve their PEC performance in the removal of pharmaceutical pollutants in wastewater. Typical studies presented involve the doping of ZnO, the synthesis of $LaFeO_3$ perovskite and the preparation of S scheme ZnO/Bi_3TaO_7 heterojunctions for PEC degradation of antibiotics in synthetic and real wastewater.

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Interfacial engineering of perovskite-structured $NiSe_2$ and $SrTiO_3$ for photoelectrocatalytic applications for norfloxacin degradation and hydrogen generation in wastewater

Idowu D. Adegbenga[a,b] *Oluchi V. Nkwachukwu*[a,b] *Omotayo A. Arotiba*[a,b,*]

[a] *Department of Chemical Sciences, University of Johannesburg, Doornfontein, 2028, South Africa*
[b] *Centre for Nanomaterials Science Research, University of Johannesburg, South Africa*

Keywords: $NiSe_2$, $SrTiO_3$, Z-scheme heterojunction, oxygen evolution and hydrogen evolution reactions, photoelectrocatalysis

Towards the engineering of semiconductors for a dual-functioning photoelectrocatalyst in environmental remediation and green energy solutions, FTO- $NiSe_2$, $SrTiO_3$, and $NiSe_2$–$SrTiO_3$ heterojunctionswere synthesized using hydrothermal method for photoelectrocatalytic (PEC) degradation of norfloxacin in real wastewater and water splitting [1]. The prepared samples were characterized using XRD, FE-SEM/EDX and HRTEM. The XRD spectra show that $NiSe_2$ and $SrTiO_3$ exhibited cubic crystal structures with space group pa-3 and pm-3m respectively. The PEC performance of the photoanodes were evaluated using norfloxacin and the results showed 90%, 80% and 34% for $NiSe_2$-$SrTiO_3$, $SrTiO_3$, and $NiSe_2$ respectively. The heterojunction showed highest degradation rate as compared to the pristine. This is attributed to more efficient light absorption and charge separation as shown from electrochemical impedance spectroscopy and linear sweep voltammetry (LSV) data. The scavenger study shows that superoxide radical ($O_2^{\cdot -}$) and hydroxyl ($^{\cdot}OH$) radical are the major species participated in PEC degradation and the heterojunction showed better stability from reusability and photoelectrochemical test. The hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) were studied using LSV to determine the photocurrent density. For the HER at 0.20 V NHE, the photocurrent density exhibited by $NiSe_2$, $SrTiO_3$, and $NiSe_2$–$SrTiO_3$ were 0.499, 0.00359, and 0.680 mA/cm^2 respectively, while for the OER at 1.5 V NHE, the photocurrent density displayed are 3.052, 0.0168, and 6.760 mA/cm^2 for $NiSe_2$, $SrTiO_3$, and $NiSe_2$–$SrTiO_3$ respectively. The heterojunction has the lowest Tafel slope, indicating a faster rate of reaction than the pristine. The heterojunction performance could be attributed to the synergistic role from both materials, improved band alignment which resulted in better charge transfer and suppression in recombination of charge carriers [2]. From the calculated band edge potentials and the scavenger studies, a Z-scheme mechanism charge transfer was proposed. In this study, the $NiSe_2$–$SrTiO_3$ heterojunction show potential for photoelectrocatalytic degradation and green hydrogen generation.

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Electrocatalytic potentials of biochars derived from *Dioscorea bulbifera* peel for hydrogen evolution reactions− experimental and tight binding quantum chemical study

Edith C. Unoka[*a,b], *J.U. Iyasele*[b], *I.E. Uwidia*[b], *Kevin Lobb*[c] *and Nnaemeka Nnaji*[*d,e]

[a]Department of Chemistry, University of Benin, Benin−City, Edo State. [b]Department of Chemical Sciences, Dennis Osadebay University, Asaba, Nigeria. [c]Chemistry Department, Rhodes University, Makhanda, Eastern Cape, South Africa. [d]Department of Chemistry, Alex Ekwueme Federal University Ndufu Alike Ikwo, Ebonyi State−Nigeria.
[e]Centre of Excellence in Carbon Based Fuels, School of Chemical and Minerals Engineering, North−West University, Potchefstroom, 2531, South Africa

Keywords: *Dioscorea bulbifera* seed peel, tight binding calculations; biochar; hydrogen evolution reactions

This study reports the electrocatalytic characteristics of biochars prepared from *Dioscorea bulbifera* seed peel for hydrogen evolution reactions (HERs) through the electrochemical and tight binding quantum chemical study. The biochars obtained through pyrolysis at 300 ºC and 400 ºC, were subjected to chemical activation to obtaine DBP@BC_300 and DBP@BC_400 respectively. The physicochemical properties of the activated biochars was evaluated using FTIR spectroscopic and BET surface area measurements. The electrocatalytic performance were evaluated using double layer capacitance values (C_{DL}) from cyclic voltammetry (CV), Tafel slopes from linear sweep voltammetry (LSV) and charge transfer resistance (R_{CT}) from electrochemical impedance spectroscopy (EIS) in different pH media. GFN2-xTB computational technique was adopted to determine the energy gap (ΔE) and Fermi energy level values of the proposed biochar models. The biochar derived electrocatalysts studied showed varying degrees of electrocatalytic performance in acidic, alkaline and neutral electrolyte solutions. DBP@BC_300 °C gave C_{DL} values of 2.6mF, 2.7mF and 2.8 mF in alkaline, neutral and acidic pH respectively and DBP@BC_400 °C gave C_{DL} values of 5.5 mF, 4.5 mF and 4.0 mF in alkaline, neutral and acidic pH respectively. These suggest that DBP@BC_400 gave the best electrocatalytic performance for HER in alkaline pH. The CV derived results are in excellent agreement with LSV result for DBP@BC_400 with the smallest Tafel slope value of 69.2mVdec^{-1} and EIS gave charge transfer resistance (R_{CT}) of 90.00 Ω value, both in alkaline pH. S**trong negative correlations were determined between** Fermi energy and C_{DL}, R^2 = 0.968 and 0.7185 respectively for DBP@BC_300 and DBP@BC_400. GFN2-xTB calculations reveals that the DOS curves at the fermi energy level were **not at zero** for both studied electrocatalyst biochar materials. This indicates the presence of electronic states available at the Fermi energy level, which enhanced easy charge transfer during hydrogen evolution reactions, and better electrocatalytic performance. Our results suggest that DBP@BC_300 and DBP@BC_400 possess good potentials for hydrogen evolution reaction electrocatalysis.

Moringa oleifera and *platanus acerifolia* capped silver nanoparticles as green nano-adsorbents for the removal of pharmaceuticals in wastewater

Precious Mahlambi and Nonhlazeko Nxumalo

Department of Chemistry, University of KwaZulu Natal, King Edward Road, Scottsville, Pietermaritzburg, 3209, South Africa, E-mail: Mahlambip@ukzn.ac.za

Keywords: Adsorption, pharmaceuticals, wastewater, low-cost adsorbent

Pharmaceuticals are one of the most prevalent contaminants discovered in water systems [1]. This prevalence has been identified to be due to the ineffectiveness of traditional wastewater treatment procedures to completely remove them and thus they are released into the rivers with the effluent water. Consequently, demanding the urgent need for efficient removal of pharmaceuticals via alternative techniques [2]. Utilizing affordable technologies while preserving safety and health standards is one of the biggest issues in the field of wastewater treatment. One of the most promising methods is the removal of pharmaceuticals using adsorption since it can be easily integrated into the present water treatment systems. In this study, *platanus acerifolia (LPL)* and *moringa oleifera* (MO) capped silver nanoparticles were synthesized as adsorbents for removing, sulfamethoxazole, nevirapine and ibuprofen pharmaceuticals in wastewater. The transmission electron microscopy result revealed the AgNps to be spherical in shape with average size of 5-10 nm, while XRD confirmed a face centered cubic crystalline nanoparticles. The adsorption experimental data showed that the nano-adsorbents fitted with the Langmuir isotherm model which indicates that the binding occurred on the homogeneous surface. Furthermore, the LPL-AgNps adsorption capacities of the pharmaceuticals were higher compared to MO-AgNps due to the LPL-AgNps larger surface areas which further enhanced the adsorption capacity. The pseudo-second-order kinetic model best fitted which implied adsorption through chemisorption, while the thermodynamic results revealed that the adsorption process was spontaneous and endothermic. The results confirmed the high efficiency and applicability of green-synthesized nano-adsorbents in the removal of S phthalate esters, Nvp and Ibu in wastewater.

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Rhizobia inoculation: a sustainable drought tolerance mitigation strategy for *Lessertia frutescens*

Mokgadi M Hlongwane[a], *Ntebogeng S Mokgalaka-Fleischmann*[a,b], *Felix D Dakora*[a]

[a]Department of Chemistry, Tshwane University of Technology, Private Bag X680, Pretoria, 0001, South Africa
[b]Faculty of Science, Tshwane University of Technology, Private Bag X680, Pretoria, 0001, South Africa
*Corresponding author: HlongwaneMM@tut.ac.za

Keywords: medicinal plants conservation, metabolites, molecular networking, sustainable agriculture

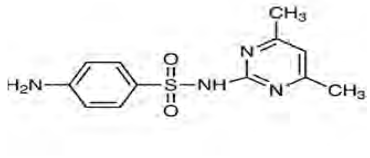
Lessertia (L.) frutescens, a valuable South African medicinal plant, is increasingly threatened by drought, which hinders its growth and phytochemical composition. This study investigated three rhizobia isolates as drought stress mitigation strategies for *L. frutescens*. *Lessertia frutescens* seedlings inoculated with isolates TUTLFNC33, TUTLFNC37 and TUTLFWC74 were subjected to three different levels of simulated drought for three months. Upon harvest, relevant measurements were performed to quantify yield, total flavonoid compounds, total phenolic compounds, DPPH radical scavenging ability and ferric reducing antioxidant potency. Additionally, semi quantification of sutherlandins A-D and sutherlandiosides A-D was conducted using LC-MS and the data processed using GNPS Classical Molecular Networking. The yield, total phenolic and flavonoid contents, as well as antioxidant activities (DPPH and FRAP) in seedlings inoculated with TUTLFNC37, were significantly higher in comparison to TUTLFNC33, TUTLFWC74, positive control and uninoculated seedlings. Molecular networking of sutherlandins A-D and sutherlandiosides A-D further revealed unique and diverse chemical profiles associated with TUTLFNC37, indicating metabolic pliability under drought. The enhanced antioxidant capacity in inoculated seedlings suggests improved oxidative stress management owed to rhizobia inoculation. These findings highlight the beneficial role of rhizobia in inducing the phytochemical defense mechanisms of *L. frutescens* under abiotic stress. The study provides insights into sustainable strategies for conserving medicinal plant species and improving their resilience to arid environments.

Exploration of aromatic plant-based materials as bio-adsorbents for the removal of pharmaceutical contaminants from wastewater

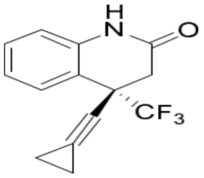
Thandeka Mbatha[a], *Precious Mahlambi*[a], *Sihle Mngadi*[b] *and Sandisiwe Zondo*[b]

[a]Department of Chemistry, University of KwaZulu Natal, Private Bag X01, Scottsville, Pietermaritzburg 3209, South Africa, E-mail: 220006971@stu.ukzn.ac.za

Keywords: Antiretroviral drugs, antibiotics, batch adsorption, adsorption efficiency, *Lippia javaniva leaves*



Sulfamethazine



Efavirenz

Antibiotic and antiviral contamination in water is currently an urgent environmental concern, necessitating effective, yet affordable water mitigation strategies. This study therefore, explored a novel batch adsorption process incorporated with raw, glycine and sodium bicarbonate modified *Lippia javanica* leaves as bio-adsorbents to decontaminate efavirenz and sulfamethazine from wastewater. SEM and FTIR images revealed that sodium bicarbonate ($NaHCO_3$) modified *Lippia javanica* had a comparatively enhanced surface porosity and more reactive surface functional groups than glycine and raw *Lippia javanica*. Sample pH, concentration and contact time were the main assessed optimization parameters to achieve an effective adsorption method. According to statistical ANOVA findings, contact time had the highest % contribution effect on the effective adsorption of efavirenz and sulfamethazine in the ranges of 76.70 % (raw bio-adsorbent) > 64.93 % (sodium bicarbonate modified bio-adsorbent) > 51.36 % (glycine modified bio-adsorbent). The adsorption rate mechanism of both compounds was best fit for a pseudo-second order model. Interestingly, the adsorption mechanism of adsorbates for functionalized bio-adsorbents followed Freundlich isotherm whilst for raw biomaterial, followed Langmuir isotherm model. $NaHCO_3$ modified *Lippia javanica* showed the highest effectiveness followed by glycine modified *Lippia javanica* and raw *Lippia javanica* with maximum adsorption capacity (q_{max}) ranging from 7.78-46.88 mg/g > 9.403-27.37 mg/g > 2.49-21.82 mg/g, respectively.

Development of KOH-activated carbon from sawdust for cosmetic dental applications

Sinenhlahla Thethwayo [a], *Yolanda Tancu* [b], *Florence Lehusto* [b], *Bhekumuzi Gumbi* [a] *

[a] *University of KwaZulu-Natal, School of Chemistry and Physics, Westville, Durban,4000, South Africa*
[b] *CSIR, Water Research Centre, Meiring Naude Road, Pretoria, 0001, Pretoria, South Africa*
218005079@stu.ukzn.ac.za

Keywords: Teeth whitening, Porous activated carbon, Sawdust

Sawdust, a prevalent byproduct of wood processing, poses serious environmental and health risks when improperly managed[1]. Unregulated storage can lead to significant pollution, and exposure to wood dust is associated with adverse health effects, including an elevated risk of respiratory diseases and cancers. Conventional disposal methods, such as combustion, release hazardous pollutants, underscoring the urgent need for sustainable waste management strategies[2]. One innovative solution is the conversion of sawdust into activated carbon, which is characterized by a high specific surface area and porosity. The production of activated carbon can be achieved through both physical and chemical activation processes. Notably, the chemical activation using potassium hydroxide (KOH) has been shown to yield highly microporous activated carbons with a specific surface area reaching up to 1876.16 m^2/g[3]. The resulting activated carbon exhibits significant potential in various applications, including oral care, particularly in teeth whitening. As consumer demand shifts towards natural alternatives from traditional whitening products, activated charcoal has gained popularity due to its efficacy in adsorbing stains and discolorations from dental surfaces. This capability is attributed to its extensive surface area and porosity, which facilitate the adsorption of pigments and chromophores[4]. The study will elucidate the dual potential of biomass-derived activated carbon as a sustainable energy source and a safe, effective agent for enhancing dental aesthetics. By addressing the environmental challenges associated with waste management and offering a natural alternative for teeth whitening, this research highlights the innovative utilization of biomass resources for both energy production and health benefits.

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A comprehensive literature review on hazardous materials in buildings

Prisca Simbanegavi[a], *and Nthabiseng Maledi*[b]

[a]School of Construction Economics and Management, University of the Witwatersranad, Johannesburg, , South Africa,
E-mail: prisca.simbanegavi@wits.ac.za.
[b]School of Chemical and Metallurgical Engineering, University of the Witwatersrand, Johannesburg, South Africa,
E-mail: nthabiseng.maledi@wits.ac.za

Keywords: asbestos-containing materials (ACMs), radon gas, polychlorinated biphenyls (PCBs), chlorofluorocarbons (CFCs), hydrochlorofluorocarbons (HCFCs), halons, lead-based paint, formaldehyde health and environmental risks

The continued presence of hazardous substances in the built environment that include asbestos-containing materials (ACMs), radon gas, polychlorinated biphenyls (PCBs), chlorofluorocarbons (CFCs), hydrochlorofluorocarbons (HCFCs), halons, lead-based paint, and formaldehyde poses significant health and environmental risks. These substances have been linked to diseases such as lung cancer, neurological impairments, respiratory conditions, and environmental degradation [1], [2]. Despite global regulations, many existing structures still contain toxic materials. Vulnerable populations, particularly children and those in low-income settings, remain disproportionately exposed to these pollutants, raising serious public health and equity concerns ([3], [4], [5] . This study aims to conduct a comprehensive literature review of the sources, pathways, health effects, and regulatory responses concerning key hazardous building materials, with a particular focus on ACMs, radon, PCBs, CFCs, HCFCs, halons, lead-based paint, and formaldehyde gas. Using a systematic literature review approach, this paper synthesises peer-reviewed journal articles, international environmental health agency reports, and policy documents published between 2000 and 2024. Studies were selected based on relevance, scientific rigour, and coverage of both human health and environmental impact dimensions. The review confirms that radon is the second leading cause of lung cancer globally after smoking [1]. PCBs have been found to disrupt neurological and developmental processes, particularly in foetuses and young children [4] . CFCs and halons are major contributors to ozone layer depletion, while exposure to lead and formaldehyde is associated with cognitive deficits, respiratory irritation, and carcinogenic effects [2], [6]. There is a pressing need for targeted policy interventions, mandatory building audits, the retrofitting or safe removal of hazardous materials, and increased public awareness. Furthermore, regulations must be strengthened and enforced to protect human health and promote sustainable building practices, particularly in aging and informal housing sectors.

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Technical development of passive samplers for environmental risk assessment with phthalate esters in water as model compounds

Ntombifuthi Mthembu[a]*,Luke Chimuka* [a] *and Ivan Hofsajer*[b]

[a]Department of Chemistry, University of the Witwatersrand, Private Bag X3, Johannesburg 2050, South Africa, E-mail: 2127438@students.wits.ac.za. [b]School of Electrical and Information Engineering, University of the Witwatersrand, Private Bag X3, Johannesburg 2050, South Africa

Keywords: passive samplers, phthalate esters, water monitoring

Phthalate esters (PAEs) are ubiquitous pollutants in water environments that continue posing significant environmental and health concerns. Passive sampling techniques have emerged as valuable tools for water monitoring, offering advantages such as cost-effectiveness, ease of deployment, and ability to detect trace concentrations. However, current passive samplers are vulnerable to theft and vandalism, particularly in developing countries, limiting their effectiveness. This project addresses this limitation by developing the technically improved passive sampler deployment systems for water monitoring, with PAEs as model compounds. Herein, we present the design and development of improved deployment passive sampler systems. Different passive sampler deployment systems were designed and tested in the Emmarentia and Hennops rivers in Gauteng.

In this study, a method for analysing selected phthalates esters, including Dimethyl phthalate (DMP), Diethyl phthalate esters (DEP), Diisobutylphthalate (DiBP), Di-n-butyl (DnBP) phthalate, Butyl Benzyl phthalate (BBP), Bis(2-ethylhexyl)phthalates (DEHP) and Di-n-octly phthalate (DnOP) was also developed using gas chromatography equipped electron capture detection (GC-ECD), achieving limits of detection (LOD) ranging from 3.89-11.2 µg/L and limits of quantification (LOQ) ranging from 12.98-37.43 µg/L.

Laboratory calibration of passive samplers for PAE uptake yielded kinetic uptake rates ranging from 0.00101 to 0.00969 L/day, with sampler-based LODs and LOQs of 0.0161-0.29 µg/L and 0,0539-0.973 µg/L respectively. Solid-phase extraction (SPE) was optimized for grab samples to compare with the passive sampling approach, yielding recoveries between 50% and 118%. Finally, Chemcatcher passive samplers, assembled with ethyl acetate membranes and C18 disks, were deployed in water bodies across the Northwest agricultural zone to assess phthalate ester contamination in the region.

Adsorptive desulfurization of diesel fuel using activated carbon from waste biomass (*Carica papaya*-PVA)

Beatice Makasi[b], Yali Yao[b], Linda Jewell [a], Liberty Mguni[b]

[a] *Department of Chemical Engineering, University of South Africa, 29 Pioneer Avenue and Christian De Wet, 1710, Florida, Private bag X6, South Africa, E-mail: 19218079@mylife.unisa.ac.za* . [b] *Institute for Catalysis and Energy Solutions*

Keywords: Waste biomass, Activated Carbon, Synthesis, Model Diesel, Adsorbent, Adsorptive Desulfurization, Adsorption capacity, MOFs, DBT.

The use of fossil fuels in transportation and industrial sectors contributes significantly to the world's economy. However, the combustion of these fossil fuels also results in the emission of various air pollutants such as sulfur oxides, which results in acid-rain by reacting with the air moisture, photochemical smog, which is detrimental to human health and the environment, corrosion problems in pumping, pipeline, and refinery equipment due to the oxyacid formation and catalytic poisoning of converters in automotive engines [1]. Deep desulfurization of these fuels is of paramount importance to support the UN Sustainable Goal 7 and Goal 15 on affordable clean energy and climate action. Adsorptive desulfurization has shown to be the most environmentally friendly, cost effective, simple and efficient method for deep desulphurization as compared to conventional Hydrodesulfurization (HDS), which utilizes expensive oxidants [2].

ADS utilises different types of adsorbents which include zeolites, activated carbons (AC), metal-organic-frameworks (MOFs). The application of AC for adsorptive desulfurization offers a solution to one of the pressing global issues regarding environmental pollution. Activated carbon (AC) has gotten lots of research attention due to its steady adsorption performance, superior mass transfer, cost effectiveness, different pore sizes (microporous, mesoporous and macropores) for adsorption of various sulphur compound sizes, large surface area for ample reactions to occur. Activated carbon (AC) from renewable and low-cost waste biomass is economical and prevents environmental degradation. [3].

This research focused on the synthesis of a low-cost adsorbent and the feasibility of activated carbon from *Carica Papaya* biomass for adsorptive desulfurization with polyvinyl alcohol (PVA) as a support/oxidise the activated carbon to increase its surface acidity towards organo-sulfur compounds. Characterization techniques such as FTIR (For functional groups), SEM (pore size distribution), BET (surface area) were used. Batch adsorption for desulphurisation was utilised to study the efficiency of DBT removal with varying adsorbent ratios, contact time also the isotherms and kinetics of the adsorption capacity was also studied.

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Chemical characterization and quantification of selected heavy metals from sand river

Salphy Monama[a], *Vusimuzi Mulaudzi*[a] *and Lutendo Macevele*[a]

[a] Department of Chemistry, University of Limpopo, Private Bag X1106, 0727, South Africa Email: salphymonama@gmail.com

Keywords: Anthropogenic sources, Diurnal variation, Heavy metals, ICP-OES, Seasonal variation, Statistical analysis, Sand River, Water quality

Heavy metals in freshwater systems are a growing concern due to their persistence and harmful effects on ecosystems and human health. This study evaluates the chemical characteristics and concentrations of six heavy metals—Copper (Cu), Nickel (Ni), Lead (Pb), Chromium (Cr), Zinc (Zn), and Iron (Fe) in the river influenced by municipal and industrial discharge. Sampling occurred three times daily (8 AM, 12 PM, 4 PM) across all four seasons and analysis was conducted using Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES). Results revealed clear seasonal and diurnal variations. Mean concentrations of Fe (3.24 ± 0.47 mg/L) and Zn (1.71 ± 0.39 mg/L) exceeded WHO and DWAF guidelines. The highest concentrations were found in summer afternoons, suggesting intensified human activity and evaporation. One-way ANOVA indicated significant statistical seasonal differences ($p < 0.05$) for Pb, Cr, and Ni. Strong correlations were found between Fe and Zn ($r > 0.85$), and between Cu and Pb, indicating common anthropogenic sources. Seasonal peaks of Cr (spring) and Pb (winter) suggest agricultural and domestic runoff contributions. These findings highlight the urgent need for regular water quality monitoring, stricter effluent regulations, and improved wastewater treatment technologies to mitigate environmental and public health risks.

Functionalized magnetic nano adsorbent for the remediation of pollutants from aqueous solution

Emmanuel Adisa, Saheed O. Sanni[a]*, Samson O. Akpotu*[a] *and Agnes Pholosi*[a]

[a]Department of Natural Science, Vaal University of Technology, Private Bag X021, Vanderbijlpark, South Africa, E-mail: agnesp@vut.ac.za

Keywords: Adsorption, polydopamine, tetracycline, magnetite, heavy metals

Water contamination by both inorganic and organic pollutants is an ongoing global environmental concern. Numerous approaches have been studied for the development of cheaper and more effective adsorbents. Superparamagnetic iron oxide nanoparticles are promising materials in emerging pollutants remediation due to their biocompatibility and easy surface modification. In this study, magnetic nanoparticles were synthesized via the co-precipitation method and coated with silica through the Stober route. This was followed by functionalization with zirconium for heavy metals and polydopamine for antibiotics remediation. The synthesized materials were characterized using XRD, SEM, TEM, BET surface area, XPS and FTIR spectroscopy. The adsorption kinetics were notably rapid, with the time required to reach equilibrium at 30 minutes for initial concentrations ranging from 50 to 150 mg/L, at a pH of 6 for heavy metals and pH 7 for antibiotics. The isotherm data revealed high adsorption capacities of 286.13, 446.56, 144.30 and 235.85 mg/g for tetracycline, ciprofloxacin, lead, and cadmium, respectively. Equilibrium studies indicated that the adsorption followed Langmuir isotherm for all adsorbents and was thus monolayer in nature, further analysis indicated that chemisorption was the predominant type of adsorption with ion exchange being the predominant mechanism of adsorption. The kinetic modelling revealed that the adsorption of heavy metals and antibiotics were best described by the pseudo second order model. The study overall finding indicates that the synthesized nanocomposites exhibit the highest efficiency in the remediation of organic and inorganic pollutants from aqueous solution with reusability of 3 cycles.

Speciation and fractionation of metals in the darvill wastewater works sludgeland using ultrasound-assisted single and sequential extraction procedures

Sbusiso Khuboni[a], Gletwyn Rubidge[b] and Sihle Mngadi[a]

[a]uMngeni-uThukela Water, Scientific Services Division, Laboratory Services Department, 310 Burger Street, Pietermaritzburg, 3201, South Africa, E-mail: Sbusiso.khuboni@uuw.co.za.
[b]Nelson Mandela University, Faculty of Science, Department of Chemistry, University Way, Summerstrand, Gqeberha, 6019, South Africa

Keywords: wastewater, environment, sludge, contamination,

Sewage sludge production is inevitable because of the rising rate of wastewater discharge brought on by urbanization and population growth, hence, there is the need for appropriate and effective sludge disposal and management practices. Disposal methods such as landfilling and incineration have been found to be environmentally harmful, while the irrigation of sewage wastewater sludge on agricultural land has been said to possess certain beneficial characteristics, such as nutrients addition and organic matter enhancement on the soil. Previous studies conducted at the Darvill Wastewater Works (DWWW) have focused on assessing the total concentration of metals in the soil and not assessing the bioavailable metals.

This study aimed to assess the level of potentially toxic metals (As, B, Ba, Cd, Co, Cr, Cu, Fe, Mn, Mo, Ni, Pb, Se, V and Zn) in soil (wet and dry season) situated within DWWW sludgeland in Pietermaritzburg, South Africa. To further determine their possible environmental implications (contamination factor, potential ecological risk index (PERI) and geo-accumulation indices) in the study area. Furthermore, the study utilised the use of statistical tools such as principal component analysis (PCA) and geographical information system (GIS) to assess the potential source of contamination and distribution patterns of these metals.

The elemental analysis revealed that the soils in the study area are contaminated by trace metals such as As, B, Ba, Co, Cu, Mn, Ni, Pb, Se, V and Zn. The concentration of these metals in both dry and wet seasons vary significantly, and this was due to rains and leaching during the wet season. The sequential extraction method used to evaluate the bioavailability of metals revealed that As was present at a higher level (fraction 1: 2-84%), and this could pose a potential threat to the environment including humans. Soil quality indicators revealed that some sample points have a moderate to trace contamination by metals like Cr, Mn and Zn, while others are generally moderately contaminated. The results indicated that the soil was enriched with moderate to significant levels of trace metals such as As, Cr, Mn, Mo, Ni, Pb and Zn. Overall, the PERI showed that DWWW is moderately contaminated. Statistical analysis using PCA revealed a strong interrelationship between metals such as B, Ba, Cd, Cr, Co and Ni and these possibly originate from various anthropogenic sources such as agricultural, municipal and industrial waste from landfills, while Cu, Fe, Mn, Mo, and Se could be from the chemicals used at the DWWW plant. In addition, geographical information system (GIS) spatial distribution patterns of trace metals confirmed the statistical and elementals analysis.

Darvill wastewater works must take the contamination of metal as a serious matter by not only assessing total metals, but also periodically evaluate the speciation of metals and environmental contamination of the sludgeland. It is recommended that rehabilitation techniques, such as phytoremediation, are adopted and implemented.

Microplastics in south african freshwater systems: a meta-analysis of concentrations, characteristics, and potential environmental risks

Augustine Madingwane[a], *Philani Mpungose*[a], *Zondi Nate*[a], *Adetunji Awe*[a] *and Lawrence Madikizela*[b]

[a]Department of Environmental and Occupational Studies, Cape Peninsula University of Technology, District Six, Cape Town, 7925, South Africa, E-mail: 219038481@mycput.ac.za [b]Institute of Nanotechnology and Water Sustainability, University of South Africa, Johannesburg, 2000, South Africa

Keywords: microplastics, concentrations, environmental risks, freshwater systems

Microplastics have grown into a significant environmental issue because of their widespread in aquatic ecosystems and their potential ecological and health risks. This study analyses the concentrations, characteristics and potential environmental risks of microplastics in freshwater systems across South Africa. A meta-analysis method was applied to analyse data for this research. Data from peer-reviewed articles, reports, and dissertations published from 2015 to 2024 were analysed to evaluate the trend in studies on pollution caused by microplastics in freshwater systems across South Africa over the years. The findings show that microplastics are prevalent in South Africa's freshwater systems. The mean concentrations of microplastics in freshwater systems that were reported in studies ranges from 0.0027 particles/L to 164.89 particles/L. High-density polyethylene, low-density polyethylene, polystyrene, polyethylene, polyethylene terephthalate, and polypropylene are the common microplastic polymer types found in freshwater systems across South Africa. This raise concerns these polymers can be carries of pollutants and can be harmful when ingested.

Common shapes that were reported include films/filaments, fibres, fragments, and pellets. Which indicates that wastewater discharge is one of the major sources of microplastics in freshwater systems. Sizes of microplastics ranges from <0.5 mm to 5 mm. These smaller particles can be easily ingested and inhaled resulting in detrimental effects on both humans and aquatic organisms. Green, white/transparent, yellow, pink/red, and blue are the common colours that were reported. These bright colours can be mistaken for food by aquatic organisms which will lead to effects such as inhibition of growth when ingested. The study also highlights the methodological diversity in microplastic research with bulk water sampling, filtration, digestion, density separation, Raman spectroscopy and Fourier-transform infrared spectroscopy (FTIR) emerging as the most used techniques due to their effectiveness and adaptability. However, there is still gaps with regards to research pertaining to microplastic occurrence in freshwater systems in South Africa, with most of the provinces having little research.

Given the effects microplastics have on humans and aquatic organisms, more research on microplastic pollution in freshwater systems in South Africa to gain more insight of their distribution throughout the country is needed. Therefore, this study will raise awareness about the need for more studies that analyses microplastics in freshwater systems, specifically surface water. This study will also serve as a guide for future research on microplastics in freshwater systems, specifically surface water across South Africa.

Phosphogypsum valorisation: fabrication of whisker fillers and REE recovery

Jean-Luc Mukaba[ab], *Leslie Petrik*[b] *and Tshentu Zenixole*[a]

[a]Department of Chemistry, Nelson Mandela University, P.O. Box 77000, Gqeberha 6031, South Africa.
E-mail: jeanlucmukaba@gmail.com. [b]Department of Chemistry, University of the Western Cape, Private Bag X17, 7535 Bellville, South Africa.

Keywords: Phosphogypsum, rare earths elements, recrystallisation, recovery.

Phosphogypsum (PG) is the major by-product generated during the production of phosphoric acid (PA) as described in equation 1. For each ton of PA produced, about 1.7 tons of PG can be produced as a precipitate which can contain up to 2000 mg/kg of the total rare earths elements (REEs) [1]. The need for REEs in current high tech electrical and electronic based materials is vital, and recovering these metals from waste sources such as PG is becoming a sustainable and viable approach due to low energy consumption, low waste generation, few emissions, environmentally friendliness, and economically feasibility [2]. Various approaches have been used up to date for REE recovery from PG but have been deemed either costly or uneconomical or unscalable [3]. Amongst other, recrystallization of PG showed a promising advantage due to both high REE recovery as well as the pure PG phase that can be obtained. The present research mainly explored and investigated avenues for fabrication of calcium sulphate whisker fillers with subsequent REE recovery for valorisation of PG waste.

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Green synthesis of gold bimetallic nanoparticles using *Aloe africana* extract via Python Taguchi DoE for enhanced photothermal application

Motlalepule Matswibila Miya[a,b], *Oluwatobi Samuel Oluwafemi*[a,b], *and Thabang Calvin Lebepe*[a,b]

[a]Department of Chemical Science, University of Johannesburg, Johannesburg, 2028,
South Africa. E-mail: oluwafemi.oluwatobi@gmail.com, calvyn.tl@gmail.com, miyamotlalepule97@gmail.com; [b]Centre for Nanomaterials Sciences Research, University of Johannesburg,
Johannesburg, 2028, South Africa.

Keywords: *Aloe africana*, gold bimetallic nanoparticles, Python Taguchi DoE, photothermal application

Bimetallic nanoparticles (BMNPs) are of significant interest due to their enhanced photothermal properties, which can effectively target and eliminate bacteria by generating local hyperthermia, leading to bacterial ablation when irradiated with Near InfraRed (NIR) light [1]. However, traditional methods for synthesising BMNPs often involve toxic and costly reagents, prompting research into green synthesis using plant extracts, which can serve as both reducing and stabilising agents [2]. Accordingly, this study aims to explore the green synthesis of gold-palladium (Au-Pd), gold-copper (Au- Cu), and gold-nickel (Au-Ni) BMNPs using *Aloe africana* extract via the Python Taguchi design of experiment (PTDoE) for enhanced photothermal effects. A Python Taguchi L 9 experimental design was utilised to optimise the process, saving time and cost. The three factors (alloyant metal, alloyant metal molarity, and different volume ratios) at three levels were selected to achieve optimal results characterised by higher surface plasmon resonance (SPR) absorbance, lower hydrodynamic (HD) size, polydispersity index (PDI), and zeta potential (ZP). The optimal conditions from PTDoE identified Au-Ni at 0.005 M concentration with a 1:1 ratio, predicting values of 632 nm (SPR), 0.29 (PDI), 211 nm (HD size), and-15.65 mV (ZP). Experimental results closely aligned with measured values of 624 nm (SPR), 0.156 (PDI), 196.43 nm (HD size), and -13.8 mV (ZP), demonstrating PTDoE's predictive accuracy. The synthesised BMNPs exhibited improved photothermal properties compared to gold nanoparticles (AuNPs) and remained stable for 24 h across various temperatures and media. This work showcases the potential of locally sourced plants as sustainable alternatives to expensive and toxic reducing agents traditionally used in nanoparticle synthesis. Additionally, the PTDoE approach offered a cost-effective platform with numerous tools and modules capable of optimising various parameters involved in the green synthesis of BMNPs, which can be used in supporting African economic development as part of a chemistry-driven transformation.

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Green synthesis and characterisation of palladium-doped gold nanorods using Aloe Africana leaf extracts

Karabo Kamogelo Khoza[1,2*] *; Thabang Calvin Lebepe*[1,2] *and Samuel Oluwatobi Oluwafemi* [1,2]

[1]*Department of Chemical Sciences, University of Johannesburg, P.O. Box 17011, Doornfontein, Johannesburg 2028, South Africa, E-mail: nhlamulok50@gmail.com, calvyn.tl@gmail.com*
[2]*Centre for Nanomaterials Science Research, University of Johannesburg, Johannesburg 2028, South Africa*

Keywords: Gold nanorods; *Aloe Africana*; Palladium; Stability

Gold nanorods (AuNRs) are favoured photothermal agents due to their unique surface plasmon resonances, but challenges such as high concentrations of biotoxic compounds like CTAB used during their synthesis and low photothermal conversion efficiency hinder their photothermal applications[1,2]. As a result, researchers have moved their focus to developing an effective green synthesis method that will use plants as a reducing and stabilizing agent since they are cheap, require less labour, and are readily available[3]. Furthermore, capping with noble metals, such as palladium, can improve photothermal conversion efficiency[4]. Therefore, in this study, *Aloe Africana* leaves were used to reduce a high amount of CTAB concentration during the synthesis of AuNRs and then they were doped with palladium to improve their photothermal efficiency and their stability at different temperatures and different culture media was evaluated. The as-synthesised AuNRs had an LSPR peak at 808 nm and after doping, the wavelength red-shifted to 824 nm with an increase in hydrodynamic size and an increase of 11.73 in their zeta potential, indicating the successful incorporation of palladium on the surface of AuNRs. The as-synthesised materials were stable in the different culture media over 24 hours and the doped AuNRs generated more heat upon irradiation compared to the undoped AuNRs This study demonstrated the successful doping of AuNRs with palladium using a local plant and their prospective usage as a photothermal agent.

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Green synthesis of gold nanoparticles using freeze-dried berry leaves

Waheed Saban[1], *Daniel Kpeglo*[2,3], *Malik Maaza*[2,3], *Adama Fall*[2,3]

[1]Department of Chemistry, Cape Peninsula University of Technology, 7381, South Africa,
E-mail: sabanw@cput.ac.za.
[2]UNESCO-UNISA Africa Chair in Nanoscience and Nanotechnology (U2ACN2), College of Graduate Studies, University of South Africa, Muckleneuk Ridge, PO Box 392, Pretoria, South Africa
[3]Nanosciences Africa Network (NANOAFNET), iThemba LABS-National Research Foundation, 1 Old Faure Road, Somerset West 7129, PO Box 722, Western Cape, South Africa

Keywords: green synthesis, gold nanoparticles, sensor

This study presents a green synthesis approach for gold nanoparticles utilising freeze-dried berry as bioreductants and capping agents. Potassium gold chloride was employed as the metal precursor, and the reaction was conducted under ambient conditions with pH adjustment. The phytochemical-rich extracts facilitated the reduction of ions, resulting in a visible colour change indicative of nanoparticle formation. The reaction mixture was stirred continuously for hours, and the resulting colloidal solution exhibited a deep purple hue, characteristic of surface plasmon resonance. Post-synthesis, the nanoparticles were isolated via centrifugation and dried at to preserve bioactivity. This method demonstrates a sustainable and reproducible route for nanoparticle synthesis, with potential applications in catalysis, biomedicine, and environmental remediation. The synthesised gold nanoparticles using berry and mint extracts will be fully characterised by UV-VIS, FTIR, XRD, SEM/TEM, DLS and zeta potential. The synthesised gold nanoparticles exhibit suitable physicochemical properties that make them promising candidates for integration into advanced biosensing applications, enabling sensitive and selective detection of target biomolecules.

Green synthesis and formulation of TiO_2 plant-based nanoparticles for skin cancer prevention

Harmony Mthombeni[a], *Paula Maseko*[b], *Prof Rosa Klein*[a],

[a]Department of Chemistry, Rhodes University, Drosty Road, Grahamstown, Eastern Cape, 6139, South Africa, E-mail: r.klein@ru.ac.za

Keywords: skin cancer, titanium dioxide nanoparticles, green chemistry, *Camellia sinensis*, lotion serum formulation, UV protection

Skin cancer is the most common form of cancer that is a global threat to the healthcare system, with an estimation to incline tremendously in the next 20 years if not detected at an early stage. Current treatments- surgery, chemotherapy, and radiotherapy- are often invasive, painful, and harmful to healthy cells [1]. This work explores an eco-friendly approach to skin cancer prevention through the green synthesis of Titanium Dioxide (TiO_2) nanoparticles using *Camellia sinensis* plant (green tea) extracts, followed by their formulation into a multifunctional lotion serum. TiO_2 was selected for its ability to block UV radiation, remain on the skin surface without penetration, and its established safety in food and cosmetic applications [2]. Phytochemicals were extracted via ultrasonic-assisted extraction, leveraging their anticancer, anti-inflammatory, and antioxidant properties. Titanium isopropoxide was reacted with the plant extract solution, the resulting product was dried and calcined. Characterisation via XRD confirmed the presence of crystalline anatase and rutile phases; SEM revealed aggregated spherical particles of ~25 nm with a smooth morphology; and TGA showed three weight loss events totalling ~ 18% (6%, 3%, and 9%). The nanoparticles were incorporated into a serum formulation with deionised water, glycerin, xanthan gum, saliguard BDHA, and essential oils to produce a 3-in-1 topical product aimed at UV protection and potential therapeutic activity against non-melanoma skin cancer. This study demonstrates the potential of plant-based nanotechnology in developing sustainable, safe, and multifunctional dermatological products, and lays the groundwork for forthcoming in vivo and in vitro studies.

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Hydrogen storage using gas hydrates in the presence of THF and 1,3-dioxolan: kinetics and thermodynamics measurements

Saeideh Babaee[a], *Hamed Hashemi*[a] *Rowan Wales*[a], *and Siqalo Ntshuntshe*[a]

Department of Chemical and Metallurgical Engineering, University of the Witwatersrand, Johannesburg, 2000, South Africa, E-mail: Saeideh.babaee@wits.ac.za

Keywords: Hydrogen Storage, Gas Hydrates, Promotors, THF, 1,3-Dioxolan

The development of safe, efficient, and cost-effective hydrogen storage technologies remains a critical challenge for the advancement of a sustainable hydrogen economy. Gas hydrates are being investigated as a solid-state storage medium for hydrogen, as hydrates represent a safe, compact, and environmentally friendly storage material. However, commercial-scale hydrogen storage remains unfeasible due to extremely high formation pressures and slow hydrate formation kinetics. In this study, the potential of gas hydrates as a hydrogen storage medium was investigated in the presence of thermodynamic and kinetic promoters. Specifically, the role of tetrahydrofuran (THF) and 1,3-dioxolane as co-formers was examined to enhance both the stability and improve the rate of hydrogen hydrates [1–3]. Systematic experiments were carried out to evaluate hydrate formation kinetics and equilibrium thermodynamics under varying temperature, pressure conditions, and promoter concentrations. The influence of THF and 1,3-dioxolane on induction time, gas uptake, hydrate stability, and hydrogen storage capacity was quantified. Results demonstrate that the combination of these additives significantly reduces induction time, improves gas incorporation rates, and lowers the equilibrium pressure required for hydrate formation, thereby improving overall hydrogen storage efficiency. The findings provide new insights into optimizing promoter-assisted hydrate systems, highlighting their potential as a viable hydrogen storage technology for large-scale energy applications.

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Integration of reverse electrodialysis dialysis for clean energy generation from desalination brine

Frank Asamoah Danso[a], *and Saeideh Babaee*[b]

School of Chemical and Metallurgical Engineering, University of the Witwatersrand, 1 Jan Smut Ave, Johannesburg, South Africa, E-mail: 2396028@students.wits.ac.za.

Keywords: desalination, energy security, response surface methodology, reverse electrodialysis, waste brine management

South Africa faces a dual challenge of persistent energy shortages and water scarcity; despite being bordered by oceans, large-scale desalination is limited due to high power demand and an unstable supply. Uneven freshwater distribution further intensifies competition among sectors, while desalination introduces the additional challenge of waste brine management. The aim of this study is to produce energy from brine obtained through energy-intensive desalination processes using reverse electrodialysis technology. Primary data were collected through laboratory experimentation using reverse electrodialysis (RED) systems to determine the influence of operating parameters, such as concentration, flow rate, and temperature, on performance metrics like open-circuit voltage and power density. The RED experiments demonstrated that power density and open-circuit voltage (OCV) improved with increasing concentration gradients. Low flow rates decreased performance, while optimal flow rates enhanced ion transport and decreased concentration polarization. While maintaining membrane integrity, temperature had a minor impact, marginally increasing OCV and power density. The combination of an ideal flow velocity, a high concentration gradient, and a moderate temperature produced the best power density. Concentration polarization and membrane resistance were among the system's drawbacks. The RED process was modelled and optimized to determine the effects of multiple operating parameters on responses using the statistical tool, Response Surface Methodology (RSM). This research provides empirical data on the effects of operating parameters on the performance of NaCl-based RED systems. In practice, it serves as a guide for RED system optimization, providing vital information for achieving maximum power density under realistic operating conditions. It supports the potential integration of RED in clean energy and water recovery applications, portraying its feasibility as a renewable energy technology in coastal regions.

The biosynthesis of silver nanoparticles and their applications

Neliswa Kunene, Anke Wilhelm, Elizabeth Erasmus, and Marietjie Schutte-Smith

Department of Chemistry, University of the Free State, Park West, Bloemfontein, 9301, South Africa, E-mail: 2017189016@ufs4life.ac.za.

Keywords: green synthesis, silver nanoparticles (AgNPs), South African medicinal plants, phytochemicals, biomedical applications

Nanotechnology is revolutionizing many scientific fields with novel applications in medical science, environmental science, and materials science [1]. Of its many applications, silver nanoparticles (AgNPs) are of particular interest due to their antimicrobial, anticancer, and diagnostic effects [2]. Green synthesis of AgNPs using plant extracts has emerged as a non-toxic, eco-friendly alternative to conventional chemical approaches, with the promise of a novel, non-toxic, environmentally friendly approach by utilizing phytochemicals as inherent reducing and stabilizing agents [3].

In this study, the green synthesis of silver nanoparticles using aqueous extracts of three South African plants, namely *Aspalathus linearis* (rooibos), *Burkea africana*, and *Strelitzia reginae*, is investigated. Phytochemical analysis of the extracts confirmed the presence of bioactive compounds such as flavonoids, phenolics, and tannins responsible for the synthesis of nanoparticles. The biosynthesized AgNPs were characterized by Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDS) as nanoparticles of varied shape and size, with elemental confirmation of silver. Further characterization using infrared (IR) spectroscopy, Transmission Electron Microscopy (TEM), and UV-Visible spectrophotometry is underway.

Successful synthesis of AgNPs using these local plants confirms that they are viable substitutes for more studied species. As an alternative to traditional methods, the process is environmentally less demanding, using unexploited local biodiversity. The research contributes to a growing body of work in advocating green nanotechnology and expanding the phytochemical studies of South African plants used in synthesizing nanoparticles.

The results of this research hold great promise for biomedical applications, especially in cervical cancer diagnosis and toxicity assessment. This work enables the development of low-cost, sustainable nanomaterials with practical therapeutic and diagnostic applications, advancing toward the greater goals of nanomedicine with accessibility and environmental friendliness.

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In vitro anticancer effects of green synthesized *Vigna unguiculata* pods silver nanoparticles

Wendy Nkomana[a,b], Nicole Sibuyi[b,c], Mervin Meyer[b] and Abram Madiehe[a,b]

[a]*Nanobiotechnology Research Group, Department of Biotechnology, University of the Western Cape, Private Bag X17, Bellville, Cape Town, 7535, South Africa*
[b]*DSTI/TIA Nanotechnology Platform, Department of Biotechnology, University of the Western Cape, Private Bag X17, Bellville, Cape Town, 7535, South Africa*
[c]*Health Platform, Advanced Materials Division, Mintek, 200 Malibongwe, Randburg, 2194, South Africa*

Keywords: green synthesis, silver nanoparticles, cowpea pods, anticancer activity

Cancer remains a major global health burden, with current treatments limited by several drawbacks like drug resistance and ineffectiveness in advanced stages. The use of nanotechnology led to the development of novel nanotherapeutic strategies, particularly silver nanoparticles (AgNPs) have demonstrated impressive anticancer activity due to their unique physicochemical properties. The physical and chemical synthesis methods of AgNPs are costly and rely on harmful chemicals. Green synthesis methods using agricultural waste like cowpea pods (CP) provides sustainable, affordable, and environmentally friendly alternatives. The CP-AgNPs were synthesized and characterized by UV-vis spectroscopy, Dynamic Light Scattering (DLS), and High Resolution-Transmission Electron Microscopy (HR-TEM). The CP-AgNPs had λ_{max} at 420nm. DLS revealed a hydrodynamic diameter of 64.94±4.293nm with polydispersity index of 0.2596±0.0152, while HR-TEM displayed an average core size of 10.99±2.6nm. The CP-AgNPs selectively reduced the cell viability of pancreatic cancer (Panc-1) cells, while demonstrating minimal toxicity against normal skin fibroblast (KMST-6) and prostate cancer (PC-3) cell lines. The co-treatments with CP-AgNPs and Doxorubicin at non-lethal concentrations caused reduction in cell viability of Panc-1 cells, suggesting that CP-AgNPs might have drug sensitizing effects. Further investigations are underway to understand the anti-cancer mechanism that resulted in the selectivity and drug sensitizing effects of the CP-AgNPs.

The use of green nanotechnology for the extraction of enzymatic proteins from banana plant waste

Joyce Mbuyi[a,b,c], *Brett Pletschke*[b], *Christian I. Nkanga*[c,d], *Rosa Klein*[a]

[a]*Department of Chemistry, Rhodes University, Makhanda, 6139, Eastern Cape, South Africa, E-mail: g24m0006@campus.ru.ac.cd,* [b]*Enzyme Science Programme (ESP),* [b]*Department of Biochemistry, Microbiology and Bioinformatics, Rhodes University, Makhanda, 6139, South Africa,* [c]*Centre de Recherche en Nanotechnologies Appliquées aux Produits Naturels (CReNAPN),* [d]*Department of Medicinal Chemistry and Pharmacognosy, Faculty of Pharmaceutical Sciences, University of Kinshasa, B.P. 212, Kinshasa XI, Democratic Republic of Congo*

Keywords: Banana, Enzyme, Nanoparticles, Green nanotechnology

The increase in the world's population is a major challenge in several sectors, particularly in public health, with the emergence of infectious diseases. The plant world offers a much-needed source in terms of under-exploited resources, such as banana plantation waste (biomass). As part of our study, we have focused on banana tree waste (leaves and pseudo-stems), which has been under-exploited until now, in order to explore its potential in terms of biomolecule extraction, more specifically proteins, which play a major role in the immune system and are therefore a powerful ally in the fight against pathogenic microbes [1]. We synthesized various metallic nanoparticles (MNPs) from three metal salts ($CuCl_2.H_2O$, $AgNO_3$, and $ZnBr_2$) and characterized them using various methods - UV-Vis, DLS, SEM-EDX, PXRD, and TGA. From the synthesized MNPs, we optimized the extraction of the proteins mobilized into their surface and compared the effect of each metal ion on protein extraction. The extracted proteins were quantified using the Bradford method and identified using SDS-PAGE. The MNPs showed a characteristic peak around 400 nm on UV-Vis, confirming successful formation of MNPs. Particle sizes were smaller than 100 nm and were shown to be crystalline on PXRD and SEM, and their thermostability was over 250 °C, confirming the successful synthesis of MNPs. The optimized extraction process with extracted proteins from AgNPs showed a yield of 55% - higher than that of the other MNPs. The extracted protein yield from liquid plant extracts alone was 22%. As a result, MNPs demonstrated the potential to immobilize sufficient proteins on their surface that can be easily recovered. Currently, studies are underway to establish a solid database and conduct tests on the enzymatic activities that these proteins may display in order to suggest future applications in drug discovery.

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Exploring the '2+1' coordination strategy in Re^{I}-tricarbonyl complexes bearing *N*-Donor ancillary ligands

Mmabatho Ledibane[a], *Orbett Alexander*[a]

[a]Department of Chemistry, University of the Western Cape, Private Bag X17, Bellville, 7535, Cape Town, South Africa.
E-mail: 4171482@myuwc.ac.za.

Keywords: Rhenium, Tricarbonyl, “2+1”, Schiff Base

Rhenium, as a group 7 congener of technetium, shares many of its chemical properties, making it an excellent surrogate for exploring and optimizing technetium chemistry, particularly in the development of tricarbonyl complexes. The *fac*-$[M(CO)_3]^+$ core (where M = Tc or Re) provides a robust and versatile scaffold for the design of active pharmaceuticals, owing to its kinetic stability and amenability to ligand functionalization [1, 2]. Moreover, the chemical coordination behaviour and nuclear properties render these stable *fac*-$[Re(CO)_3]^+$ complexes very versatile and suited for applications across medicinal chemistry, catalysis and radiopharmaceutical sciences [3-5].

This work focuses on the development of "2 + 1" rhenium tricarbonyl complexes of the general formula *fac*-$[Re(CO)_3(N,O\text{-Bid})(X)]$, where *N*,*O*-Bid are bidentate Schiff base ligands and X is a series of monodentate ligands with various derivatives such as pyridyl, N-heterocyclic carbene (NHC), and azide moieties.
In view of the conference theme **“A WINDOW FOR CHANGE”**, the versatile synthetic route of the [2 + 1] mixed-ligand-approach offers opportunities to optimize the properties and further find synergies via *SAR*, as this approach consists of tuneable bidentate ligand and a monodentate ligand. This serves as a sufficient rationale to further investigate with new bidentate ligands, more so when recent studies using rhenium(I) tricarbonyl complexes have shown promising results as potential anticancer agents [6].

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Re^{I}-tricarbonyl complexes with pyrazolyl-based ligands as potential anticancer metallo-drugs

Boitumelo Nthapo[a], *Orbett Alexander*[a]

Department of Chemistry, University of the Western Cape, Bellville, 7535, Cape Town, South Africa
E-mail: 4428325@myuwc.ac.za

Keywords: Pyrazole, Rhenium, Tricarbonyl Chemistry.

Global health care systems remain challenged and under pressure due to the burden of disease. Many diseases, including cancer, infectious diseases, and neurological disorders, remain challenging to treat due to drug resistance, toxicity, and lack of targeted therapies. These factors, among many others, necessitate the discovery of novel and effective agents.[1]

In recent years, there has been extensive exploration into rhenium(I) tricarbonyl chemistry, with its compounds emerging as promising candidates for antibacterial and anticancer therapies [2,3]. Molecular interactions between DNA and Re^{I} tricarbonyl complexes are particularly crucial in various significant investigations, including cancer treatment [2]. Additionally, numerous pyrazole compounds are renowned for their remarkable medical and photophysical applications [3], exhibiting potential anti-cancer, anti-bacterial, anti-parasitic, and anti-viral (HIV-1) activities [4].

In this project, our objective is to design and synthesize a variety of pyrazolyl-based ligands to form bidentate chelating frameworks. These ligands will then be coordinated with rhenium metal ions to create tricarbonyl Re^{I} organometallic complexes, capitalizing on their exceptional medicinal properties for targeted anti-cancer and anti-bacterial applications, among others. All synthesized compounds will undergo thorough analysis using techniques such as IR, UV/Vis, SC-XRD, and NMR.

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Design and synthesis of rhenium tricarbonyl complexes with tridentate nitrogen-donor ligands

Brithney Snyman[a], *Orbett Alexander*[a]

Department of Chemistry, University of the Western Cape, Robert Sobukwe Rd, Bellville, 7535, Cape Town, South Africa
E-mail: 3937506@myuwc.ac.za

Keywords: Rhenium, Cancer

Cancer is a disease characterized by the uncontrolled growth of cells caused by genetic mutations in DNA. It remains one of the leading causes of death globally and represents a major challenge to public health systems around the world [1]. In recent years, significant research has focused on the development of metal-based compounds as potential anticancer agents. Among these, complexes containing tridentate nitrogen-donor ligands have attracted particular attention. These ligands, commonly derived from pyridine and quinoline structures, can strongly coordinate with transition metals such as rhenium (Re), forming stable and bioactive complexes. Their ability to interact with important biological targets like DNA and proteins contributes to their potential as effective anticancer agents. Rhenium(I) tricarbonyl complexes with tridentate nitrogen-donor ligands have shown anticancer activity through several mechanisms, such as interacting with DNA, blocking enzymes, producing reactive oxygen species, and targeting mitochondria [2,3]. Their photophysical properties also make them useful for theranostic applications, combining both cancer treatment and imaging [4,5].

Therefore, this research project focuses on the synthesis of tridentate nitrogen-donor ligands and their coordination with rhenium to form tricarbonyl complexes. All ligands and metal complexes will be characterized using IR, NMR, UV-Vis, and SC-XRD. The aim is to develop novel compounds with potential applications in cancer treatment, contributing to advances in medicinal chemistry and healthcare.

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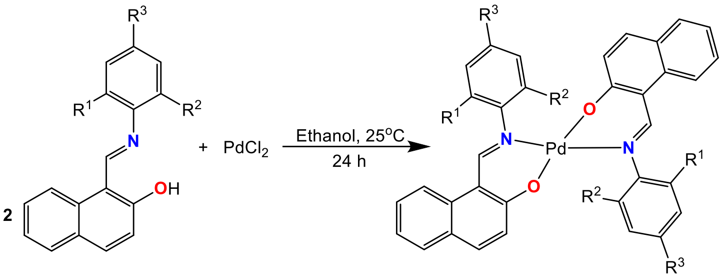
Anticancer and antibacterial potential of Pd(II) complexes derived from N_2O_2-donor bidentate Schiff bases: *in vitro* and computational studies

Segun D. Oladipo[a], *and Robert C. Luckay*[a]

[a]Department of Chemistry and Polymer Science, Stellenbosch University, Private BagX1, Matieland 7602, South Africa, E-mail: 28512928@sun.ac.za.

Keywords: Schiff Base, Palladium complex, crystal structure, anticancer, antimicrobial

A series of five palladium(II) complexes (**1** – **5**) of the formula [Pd-(**L**)$_2$] (L = (*E*)-1-(((2,6-dimethylphenyl)imino)methyl)naphthalen-2-ol(**L1**)(**1**),(*E*)-1-(((2,6-diisopropylphenyl)imino)methyl)naphthalen-2-ol (**L2**) (**2**), (*E*)-1-(((2-fluorophenyl)imino)methyl)naphthalen-2-ol (**L3**) (**3**), (*E*)-1-(((4-fluorophenyl)imino)methyl)naphthalen-2-ol (**L4**) (**4**) and (*E*)-1-(((4-bromophenyl)imino)methyl)naphthalen-2-ol (**L5**) (**5**)) were synthesized and characterised by spectroscopic techniques and physicochemical methods. Single crystal X-ray crystallography confirmed the molecular structures of complexes **3** and **4** as neutral species in which one palladium(II) centre was coordinated to two bidentate Schiff bases (**L3** and **L4**) via the imine nitrogen and naphtholate oxygen, adopting distorted square planar geometries. Quantum chemical calculations were carried out using B3LYP/3-21G DFT method and this revealed that the energy bandgap of **1** – **5** ΔE = ~3.0 eV. All the complexes showed moderate to good antimicrobial activities. Complexes **2** and **5** with MIC values of 125 µg/mL, were found to be more active than fluconazole (MIC value of 1000 µg/mL) against *Candida albicans*. Against methicillin-resistant *Staphylococcus aureus* (MRSA), complex **5** showed similar activity to gentamicin. Complex **1** was found to be more cytotoxic than cisplatin against both human cervical HeLa and human breast MDA-MB-231 cancer cell lines with cytotoxicity IC_{50} values of 22.3 ± 10.8 µM and 6.4 ± 0.1 µM respectively. Molecular docking simulation was carried out for complex **1** against cyclin-dependent kinase protein (3QTR) and serine-protein kinase (4DRH) important in cervical and breast cancer respectively and found to have improved docking scores and interactions compared to cisplatin. Complexes 2 and 5 were modelled against bactericidal targets nucleoid occlusion protein (5HSZ), chaperone (4E81), nucleoside phosphatase (7D8I) and peptidyl-propyl isomerase (5HW8) and were found to compare well against the standard drugs gentamicin and fluconazole. The findings show that complex **1** has good anticancer drug potential, while complexes **2** and **5**, are promising antibiotic leads for further pre-clinical development.



$R^1 = R^2 = Me, R^3 = H, Pd(L1)_2$, **1**
$R^1 = R^2 = iPr, R^3 = H, Pd(L2)_2$, **2**
$R^1 = R^3 = H, R^2 = F, Pd(L3)_2$, **3**
$R^1 = R^2 = H, R^3 = F, Pd(L4)_2$, **4**
$R^1 = R^3 = H, R^3 = Br, Pd(L5)_2$, **5**

Scheme 1: Synthesis of palladium(II) Schiff base complexes **1- 5**

Synthesis and application of novel Ga_2O_3-based heterostructure photocatalysts for photocatalytic nitrogen reduction

Rendani J. Mudau,[a], *Alli A. Yakubu*[b] *and Jaco Olivier*[b] *and Adeniyi S. Ogunlaja*[b]

[a] Department of Chemistry, Nelson Mandela University, Summerstrand, P.O. Box 77000, Port-Elizabeth, South Africa, E-mail: s225615231@mandela.ac.za.

Keywords: Ammonia, Fixation, $Ga_2O_3@Bi_3O_4Br$, Hydrogen, Photocatalysis

Hydrogen energy has high efficiency, environmentally friendly, lacks carbon emissions and has wide range of applications. However, it is expensive to store and transport (hydrogen) H_2, hence the need to convert to ammonia (NH_3). Ammonia can meet the demand for storing energy in time and in space (energy export and import) due to its stability for long-term storage and at low storage pressure, and ability to hold up to three atoms of hydrogen [1]. Haber-Bosch process has been widely used to convert N_2 to NH_3, however the method results in greenhouse gas emissions due to the high stability of N_2 molecules (N≡N bond energy 941.3 kJ mol^{-1}) [2]. Herein, a novel photocatalysts, ($Ga_2O_3@Bi_3O_4Br$, $Ga_2O_3@Bi_2MoO_6$, and $Ga_2O_3@Bi_2Te_3$) metal oxides were synthesised hydrothermally and employed for photocatalytic reduction of N_2. % of Ga_2O_3 was in-situ grown around Bismuth, forming compact (3%, 5%, 10% and 15%) $Ga_2O_3@Bi_3O_4Br$, $Ga_2O_3@Bi_2MoO_6$, and $Ga_2O_3@Bi_2Te_3$). The catalysts were then characterised X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Energy Dispersive X-Ray Analysis (EDX), UV-Vis diffuse reflectance spectroscopy (UV-Vis-DRS), Fourier-transform infrared spectroscopy (FTIR), Mott-Schottky plots, Scanning Electron Microscopy (SEM), Elemental mapping and High-Resolution Transmission Electron Micrograph (HRTEM). Products were analysed using Nessler's and Berthelot's reagent.

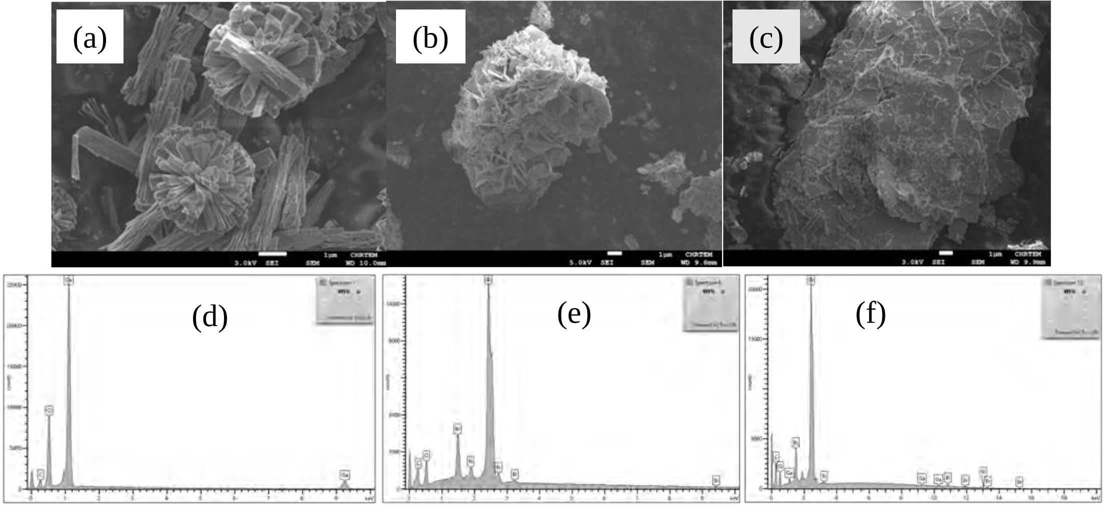


Figure 1: (a, b, c) SEM image of $\beta-Ga_2O_3$, Bi_3O_4Br, 15%$\beta-Ga_2O_3@Bi_3O_4Br$ and (d, e, f) EDS of $\beta-Ga_2O_3$, Bi_3O_4Br and 15%$\beta-Ga_2O_3@Bi_3O_4Br$

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Synergistic enhancement of photocatalytic CO_2 reduction by induced piezoelectric effect via PVDF based heterojunctions

Musingadi Murangi,[a] *Alli A. Yakubu*,[a] *and Adeniyi S. Ogunlaja*[b]

[a] *Department of Chemistry, Nelson Mandela University, Summerstrand, P.O. Box 77000, Port-Elizabeth, South Africa, E-mail: s228071925@mandela.ac.za.*

Keywords: Carbon dioxide, Heterojunction, Photocatalysis, PVDF, PVDF@Bi_3O_4Br

Carbon dioxide (CO_2) is the leading greenhouse gas, contributing about 75% to greenhouse emissions [1]. It is primarily released through respiration and fossil fuel burning [2]. Since 1750, atmospheric CO_2 levels have risen from 278 ppm to 419.3 ppm in 2023, mainly due to fossil fuel combustion for transport, electricity, and industry [3]. Photocatalysis offers a promising, sustainable method to convert CO_2 into valuable chemicals and fuels using light energy, helping to mitigate increasing CO_2 levels and their environmental impacts. Herein, a series of novel PVDF-based nanocomposites and heterojunctions were synthesized using electrospinning and hydrothermal methods and employed for photocatalytic reduction of CO_2. The catalyst was then characterised using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Energy Dispersive X-Ray Analysis (EDS), Thermogravimetry Analysis-Differential thermal calorimetry (TGA-DSC), UV-Vis diffuse reflectance spectroscopy (UV-Vis-DRS), Fourier-transform infrared spectroscopy (FTIR), Scanning Electron Microscopy (SEM) and Photoluminescence (PL). The XRD pattern of PVDF showed dominant β-phase peak at 2θ values (planes) 19.59° (110) and α-phase peaks at 16.51° ((100)) and 29.69° ((021)), (Fig 1(a)). For PVDF@Bi_3O_4Br, characteristic peaks were observed at 2θ values (planes) of 28.65° (121), 33.44° (022), and 34.79° (200), confirming the incorporation of the Bi_3O_4Br (Fig 1(a)). For PVDF@β-Ga_2O_3 characteristic peaks observed at 2θ values (planes) of 29.69° (110), 35.52° (111), and 37.18° (002) are attributed to the monoclinic β-phase of gallium oxide (β-Ga_2O_3) (Fig 1(a)). SEM images in Fig.1 (b,c) revealed that pure polyvinylidene fluoride (PVDF) exhibit fibrous structure often containing beads. Upon the incorporation of Ga_2O_3, Fig.1 (d,e) shows that while the fibrous morphology was retained, Ga_2O_3 particles were observed embedded on the PVDF surface, with beads also present. EDS data, summarized in Table 1, confirmed the successful synthesis and elemental composition of the composites. This work presents new insight into fabricating step-scheme PVDF based heterojunctions.

Table 1: EDS of PVDF and its composites.

Elements	PVDF	PVDF@Bi_3O_4Br
F	99.0	72.2
Ga	0.0	0.0
O	0.0	17.3
Bi	0.0	4.0
Br	0.0	2.7
Au	1.0	2.2

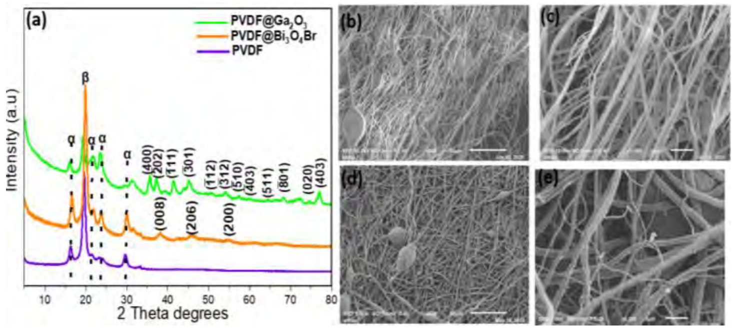

Figure 1 shows (a) the XRD patterns of pure PVDF and PVDF composites, (b, c) SEM images of pure PVDF at overview and zoomed area, respectively, and (d, e) SEM images of PVDF@Ga_2O_3 at overview and zoomed area, respectively.

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Evaluating the discrimination capability of an imide-functionalized host compound toward picoline isomers

Lesedi Rambevha and Eustina Batisai

Department of Chemistry, University of Venda, Thohoyandou, 0950, South Africa, E-mail: 18002234@mvula.univen.ac.za.

Keywords: host-guest, inclusion compounds, picoline isomers, separation

Host-guest chemistry is a specialized area within supramolecular chemistry that investigates the interaction between two molecules: a larger 'host' molecule and a smaller 'guest' molecule. This interaction is made possible by weak interactions like hydrogen bonds, ionic attractions, van der Waals forces, or hydrophobic effects [1]. The host molecule is like a container with a specific area meant to fit the guest snugly, allowing for a selective and specific binding between the two [2]. The separation of picoline isomers is crucial due to their diverse applications in various industries. Each picoline isomer has unique chemical properties that make it suitable for specific applications. 2-Picoline is used in the production of herbicides. 3-Picoline is important in the synthesis of vitamins and pharmaceuticals [3]. 4-Picoline is utilized in the manufacture of agrochemicals and as a precursor for various chemical synthesis [4]. Therefore, the separation of picoline isomers is essential not only for maximizing economic returns but also for enhancing the efficiency of chemical processes and supporting environmental sustainability initiatives.

In this project, we report the synthesis of a novel host compound, 2-(1,3-dioxo-1H-benzo[de]isoquinolin-2(3H)-yl) acetic acid, designed for the selective separation of picoline isomers. The host was characterized by thermogravimetric analysis (TGA), single-crystal X-ray diffraction (SCXRD), and powder X-ray diffraction (PXRD). Its selectivity towards different picolines was evaluated through competition experiments, and the resulting inclusion complexes were further characterized using TGA, SCXRD, PXRD, and GC. The results demonstrate the host's ability to discriminate between picoline isomers, highlighting its potential for applications in efficient isomer separation and sustainable chemical processes.

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Discrimination of isomers using hosts containing an imide functional group

Nyandano Netsianda and Eustina Batisai

Department of Chemistry, University of Venda, University Road, Thohoyandou, 0950, South Africa, E-mail: 20013614@mvula.univen.ac.za.

Keywords: cavity-based binding, host-guest complex, surface-based binding, picoline isomer

Host-guest chemistry is the branch of supramolecular chemistry concerned with the study of non-covalent interactions between a host compound and a guest [1]. The host is typically a crystalline material capable of accommodating guest species either through cavity-based inclusion or surface binding. Guests are compounds that are enclosed within or bound to the cavity or the binding sites of the host compound [2]. Host compounds can be organic or metal-organic and have numerous applications, one of the most prominent being liquid separation [3]. This process includes the separation of both isomeric and non-isomeric mixtures. This study focuses on isomeric mixture separation, which presents a significant challenge due to the structural similarities of isomers. Existing methods for separating isomers are often energy-intensive, costly, and complex [4].

This study investigates the ability of imide-functionalized host compounds to discriminate picoline isomers. We report the synthesis and characterization of two organic host molecules: 2-(carboxymethyl)-1,3-dioxoisoindoline-5-carboxylic acid (Host-1) and N-Phthaloylglycine (Host-2). These hosts were exposed to mixtures of picoline isomers, and the resulting host–guest complexes were analysed using single-crystal X-ray diffraction (SCXRD), powder X-ray diffraction (PXRD), gas chromatography (GC), and thermogravimetric analysis (TGA). Hirshfeld surface analysis was also performed to quantify the intermolecular interactions within the complexes. The findings from these techniques are discussed, with a focus on the host compounds’ selectivity and preference for specific picoline isomers.

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Catalytic transformation of CO_2 to dimethyl ether via transition metal catalysis for sustainable hydrogen storage

Bafokeng Sekaleli[a], *Abdul Mahomed*[a], *Thishana Singh*[a] *and Holger Friedrich*[a]

[a] School of Agriculture and Science, Discipline of Chemistry, University of KwaZulu-Natal, Westville, Campus, Private Bag X54001, Durban 4000, South Africa. 225111039@stu.ukzn.ac.za

Keywords: Hydrogen storage, Transition metal catalysis, DME

Greenhouse gas emissions and associated climatic changes are considered one of the most serious environmental problems of our time [1]. Achieving a balance between atmospheric carbon emissions and removal is crucial to address the environmental concerns surrounding CO_2 to achieve the sustainable development goal of reaching net-zero emissions. Therefore, removing CO_2 from the atmosphere as well as moving away from fossil fuels as a source of energy are important for this goal. This can be approached in two ways: first, CO_2 can be repurposed as a single-carbon raw material (C1 feedstock) for bottom-up chemical synthesis [2]. Due to its abundance, low cost and recyclability [3] CO_2 is highly desirable in the chemical synthesis of various commodities – with the annual global consumption roughly being 110 Mt. Despite this, CO_2's high thermodynamic stability and low kinetic reactivity, owing to its highly oxidized state, pose challenges to its use as a feedstock. Second, producing hydrogen for clean energy supply as an alternative to burning fossil fuels for energy production can help reduce greenhouse emissions [4].

The limited supply of electrical energy globally necessitates the development of efficient and cost-effective solutions, such as hydrogen technology, to mitigate this growing energy crisis [5]. However, storing and transporting hydrogen as a gas or liquid is challenging. Therefore, combining CO_2 with hydrogen to produce chemicals with high volumetric energy density, such as dimethyl ether (DME), which can be liquified under mild conditions, is a good approach for hydrogen storage and transportation [6].

Our work focuses on developing and employing catalytic systems capable of activating CO_2 in reactions with hydrogen to produce dimethyl ether (DME). The one part of the catalytic system comprises of Cu, Zn, Zr supported on CeO_2. The other part of the catalytic system comprises of a zeolite (HZSM-5). In this reaction (Scheme 1), CO_2 is hydrogenated to methanol, followed by dehydration of methanol to DME. The expectation is to obtain DME in relatively low yield due to water as a by-product which limits the reaction. Unreacted methanol and carbon monoxide are also expected to be detected.

$$\text{i)}\quad CO_2 + 3H_2 \longrightarrow CH_3OH + 2H_2O, \qquad \Delta H = -\,49.5\ \text{KJ/mol}$$

$$\text{ii)}\quad 2CH_3OH \longrightarrow CH_3OCH_3 + H_2O, \qquad \Delta H = -\,23.4\ \text{KJ/mol}$$

Scheme 1: *Reaction steps in the synthesis of DME from CO_2 and H_2*

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Synthesis, characterisation and biological studies of oxovanadium(IV) schiff Base complexes of *O,N,N′*-imidazole-aminophenol and phenanthroline-derived bases

Nonhlanhla Nkosi[a], *Kristy-Lyn Barry*[a], *Matthew Akerman*[a]

Discipline of Chemistry, University of KwaZulu-Natal, Corner of Golf and Ridge Roads, Pietermaritzburg, 3201, South Africa, E-mail: 220026377@ukzn.ac.za.

Keywords: Oxovanadium(IV), Schiff base, stability

Current pharmaceutical research aims to develop more effective and less toxic anticancer drugs capable of overcoming traditional platinum drug resistance using coordination compounds of transition metals other than platinum, such as vanadium.[1-3] The mechanism of action of vanadium-based chemotherapeutics typically involves the complexes binding to DNA via intercalation followed by oxidative DNA cleavage, which induces cell apoptosis. In this work, oxovanadium(IV) has been selected as the metal centre for the design of cationic complexes. Cationic complexes enable interaction with the negatively charged sugar-phosphate backbone of DNA. 1,10-Phenanthroline (PHEN) and dipyrido[3,2-d:2',3'-f]quinoxaline (DPQ) were chosen as the co-ligands in the heteroleptic complexes based on these ligand's ability to bind to DNA.[4] O,N,N′-tridentate Schiff base ligands complete the octahedron. Cationic oxovanadium(IV) complexes of *O,N,N′*-tridentate imidazole–aminophenol Schiff Bases and phenanthroline-derived ligands have been shown to be cytotoxic against triple-negative breast, cervical and neuroblastoma brain cancer cell lines.[5] Stability studies of the complexes in biological media are an important aspect of the biological properties of oxovanadium complexes as biological activity of a complex can be improved by increasing its bioavailability through enhancing the stability of the complex. The degree of hydrolytic stability of heteroleptic oxovanadium(IV) complexes containing a *N,N*-bidentate co-ligand can vary significantly depending on the nature of the ligands coordinated, solvent media and pH. The syntheses, characterisation and stability studies in biological media of complexes of the type [VO(ONN)(NN)]PF_6/Cl where NN = PHEN (**1,2**) and DPQ (**3,4**), as shown in Figure 1 (a) are reported. DFT-calculated electronic structures (Figure 1(b)) gain insight into the structural and electronic attributes of the compounds that might impact on their stability and interaction with DNA and other biomolecules.

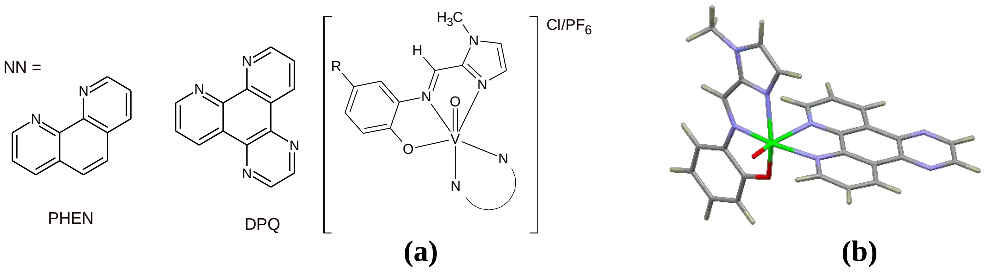

Figure 1: (a) Structures of complexes [VO(ONN)(NN)]Cl/PF_6 (R = H (**1,3**), CH_3 (**2,4**); NN = PHEN (**1,2**), DPQ (**3,4**). (b) DFT-simulated geometry-optimised structure (B3LYP/6-311G(dp) level of theory) of Complex **3**.

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Bio-derived Al_2O_3–Fe_2O_3–CaO hybrid photocatalyst for enhanced photocatalytic UV-assisted degradation of Tilmicosin

Abayomi Bamisaye[a,b*], *Nejat Habib*[b], *Kayode Adesina Adegoke*[c], *Mopelola Abidemi Idowu*[d], *and Henrietta Langmi*[b*]

[a]Department of Chemistry, Faculty of Natural and Applied Sciences, Lead City University, Ibadan, Nigeria, E-mail: abayomibamisaye@gmail.com, [b]Department of Chemistry, University of Pretoria, Pretoria, 0002, South Africa, E-mail: henrietta.langmi@up.ac.za. [c]Department of Chemical and Physical Sciences, Walter Sisulu University, South Africa. [d]Department of Chemistry, Faculty of Physical Sciences, Federal University of Agriculture, Abeokuta, Nigeria

Keywords: Photocatalysis, Tilmicosin, Nanocomposite, Biomass, Wastewater

The continuous rise in human-induced (anthropogenic) release of pharmaceutical residues into aquatic environments presents a significant environmental concern. In response, this study explores the synthesis and performance of bimetallic, biomass-derived nanocomposites as photocatalysts for ultraviolet (UV)-driven degradation of tilmicosin (TLM). The Al_2O_3-Fe_2O_3 nanocomposite was prepared using a wet impregnation technique, incorporating calcium oxide (CaO) obtained from snail shells as a sustainable precursor. Comprehensive material characterization was conducted via UV-Vis spectroscopy, X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDS). FTIR spectra of the Al_2O_3-Fe_2O_3 nanocomposite revealed a distinct absorption peak at 617 cm^{-1}, corresponding to Al–O and Fe–O vibrational bonds. XRD analysis confirmed a face-centered cubic crystalline structure, with a calculated interplanar spacing (d-spacing) of 6.75554 Å. UV-Vis results showed an absorption maximum (λ_{max}) at 335 nm and an estimated optical band gap of 3.04 eV, derived using Tauc's plot. SEM micrographs indicated the presence of rectangular to cubic-shaped aggregates, with an average crystallite size of 28.06 ± 5.19 nm. Photocatalytic testing under UV light demonstrated optimal degradation efficiencies of 86.79% and 80.69% using catalyst dosages of 0.3 g and 0.2 g, respectively. Kinetic analysis revealed that the degradation followed a pseudo-first-order reaction, with rate constants (k) of 0.0112 min^{-1} and 0.010 min^{-1} for the respective catalyst dosages. The high photocatalytic activity, simple fabrication method, and use of eco-friendly precursors highlight Al_2O_3-Fe_2O_3-CaO as a promising, low-cost photocatalyst for the effective treatment of antibiotic-contaminated wastewater.

Influence of substituents on the biological activity of Pd(II) complexes with halogen and alkyl substituted *ON* donor Schiff base ligands

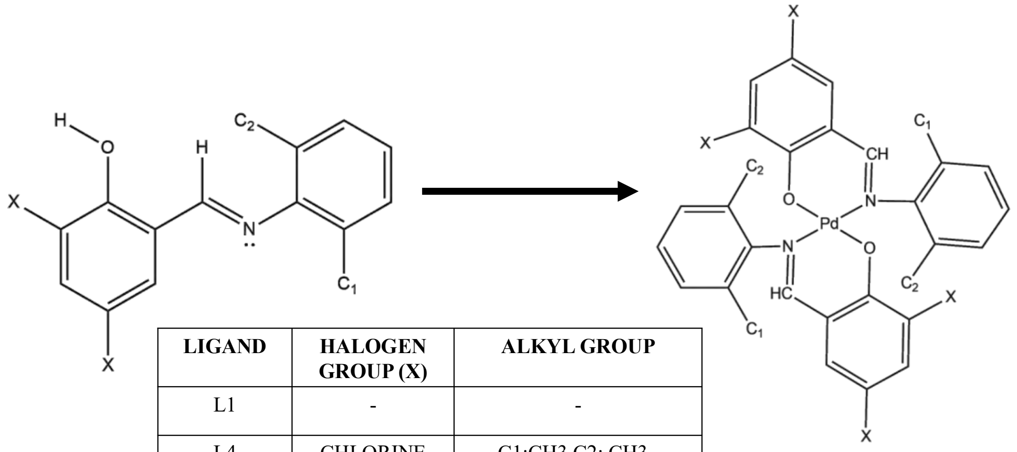
Tsholofelo Suzen Nthehang[a], *Ibrahim Waziri*[a] *and Alfred Muller*[a]

[a]Department of Chemical Sciences, University of Johannesburg, PO Box 524, Auckland Park, 2006, South Africa, E-mail:tntehang@gmail.com.

Keywords: Antimicrobial resistance(AMR), Schiff Base, Palladium, Anticancer, Antibacterial, Antioxidant

Antimicrobial resistance (AMR) is a global health predicament that impacts people from all social classes. The result of this has led to a constant rise in its mortality rate that is projected to reach the 10 million mark by the year 2050, and the World Health Organisation has since listed it in the top 10 global health threats to humanity [1]. In response to this, South Africa has developed and is currently implementing a national action plan which, among other objectives, is aimed at improving awareness, reducing the occurrence of misdiagnosis and supporting the research and development of novel drugs and medicinal solutions with potential to reduce the rise of AMR and improve treatment outcomes [2, 3]. Therefore, the aim of this study was to investigate the biological potency of Schiff base ligands and their respective metal complexes and to investigate the influence that alkyl and halogen substituents have on their pharmacological efficacy. Schiff base ligands (L1, L4, L7 and L10) were synthesised, complexed onto a Pd(II) metal centre (C1, C4, C7, and C10) and assessed for their antimicrobial, antioxidant and cytotoxic activity. The results show that compounds L4/C4 displayed the best cytotoxic potential, L10/C4 had the best antioxidant activity, and L4 & L7/C1 & C10 had the best antibacterial activity, with the *Escherichia coli* gram-negative bacteria being the most susceptible to the compounds' treatments.

Structure Block/Scheme



LIGAND	HALOGEN GROUP (X)	ALKYL GROUP
L1	-	-
L4	CHLORINE	C1:CH3 C2: CH3
L7	BROMINE	C1: H C2:CH(CH3) $_2$
L10	IODINE	C1:H C2:C (CH3)$_3$

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Intrinsic defects of lithium and sodium co-doped Cu_2ZnSnS_4 kieserite for application as counter electrons in solar cells application. First-principle calculations.

Seiso E. Tsoeu[1]*, Molepo Mahlaga,. Nosipho Moloto*[1]

Department of School of Chemistry, University of the Witwatersrand, Private Bag 3, Wits 2050, South Africa
Department of School of Physics, University of the Witwatersrand, Private Bag 3, Wits 2050, South Africa
557872@students.wits.ac.za or Seisotsoeu@gmail.com

Keywords: Density functional theory; Cu_2ZnSnS_4; $LiZnSnS_4$ doped, $NaZnSnS_4$-doped

This study evaluated the electronic structure and optical properties of Cu_2ZnSnS_4, Li-doped, Na-doped, and (Li, Na) co-doped Cu_2ZnSnS_4 using the first-principles pseudopotential plane-wave approach based on the density functional theory method [1]. The obtained electronic band gap showed a reduction form of Cu_2ZnSnS_4, $LiZnSnS_4$ doped, $NaZnSnS_4$ doped respectively. (Li, Na)- Cu_2ZnSnS_4 co-doped has great real conductivity compared to $LiZnSnS_4$ doped, $NaZnSnS_4$-doped and pure Cu_2ZnSnS_4, showing highest efficiency for solar cells.

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Nickel(II) pyrazole-pyridine complexes as catalysts for transfer hydrogenation of quinoline

Rotondwa Mphephu,[a] *Andrew J. Swarts*[a]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa
Email: 1938482@students.wits.ac.za

Keywords: Ammonia borane, Ni(II) complexes, transfer hydrogenation, quinoline

With modern sustainable chemistry, new catalytic processes have been developed that allow chemical transformations to take place under mild, clean conditions with high efficiency. The hydrogenation process is a major transformation in scientific research, and it is extensively used in pharmaceutical synthesis [1-2]. A wide range of pharmaceutical and agrochemically important compounds can be formulated using 1,2,3,4-tetrahydroquinoline derivatives, which are also found in many natural products [3-4]. Herein we report the synthesis of Ni(II) Pyrazole-Pyridine complexes bearing different steric properties for transfer hydrogenation of quinolines using ammonia borane (AB) as hydrogen (H_2) source (**Figure 1**). Catalytic performance was screened under various conditions, with optimization studies revealing methanol as the most effective solvent. Under mild conditions, using only 1 mol% of the Ni(II) complex, over 80% conversion of quinoline to 1,2,3,4-tetrahydroquinoline was achieved within 30 minutes. Results from this study demonstrate how earth-abundant nickel catalysts perform in hydrogen transfer reactions, providing an alternative to noble metals that is both cost-effective and sustainable.

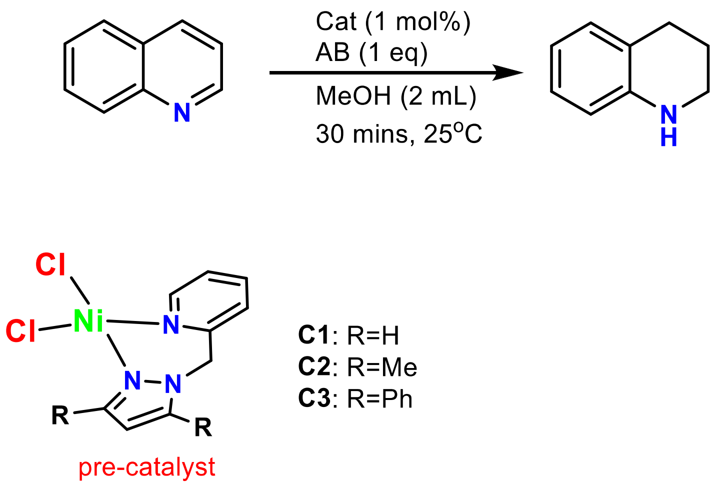

Figure 1: Transfer hydrogenation of quinoline catalysed by Ni(II) Pyrazole-Pyridine complexes

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Photodynamic antitumor and antimicrobial activities of Sn(IV) tetra(pentafluorophenyl)bacteriochlorins

Kaisano G. Tauyakhale, *Mahlatse M. Ledwaba, John Mack and Tebello Nyokong*

Institute for Nanotechnology Innovation, Rhodes University, Makhanda 6140, South Africa, E-mail: j.mack@ru.ac.za

Keywords: Photodynamic therapy, Photosensitizer dyes, Porphyrins, Bacteriochlorins, Photophysics

Photodynamic therapy (PDT) is an emerging treatment that combines photosensitizer dyes, light, and oxygen to selectively obliterate cancerous cells [1-2]. In this study, novel pentafluorophenyl-substituted porphyrinoids and their bacteriochlorin (BChls) analogue dyes were synthesised, purified and characterised, then applied. These photosensitizers were tailored to absorb well within the therapeutic window region (620−850 nm) for deep cell penetration when activated by light of a specific wavelength [3]. Moreover, the reduction of porphyrins into BChls improves solubility, high oxygen quantum yields, long triplet lifetimes and most importantly, nontoxic and rapid clearance out of the body after therapy, unlike other FDA-approved PS drugs such as Photofrin, Levulan, Metvix and Photochlor [4-5]. **Figure 1** below shows the porphyrinoids studied.

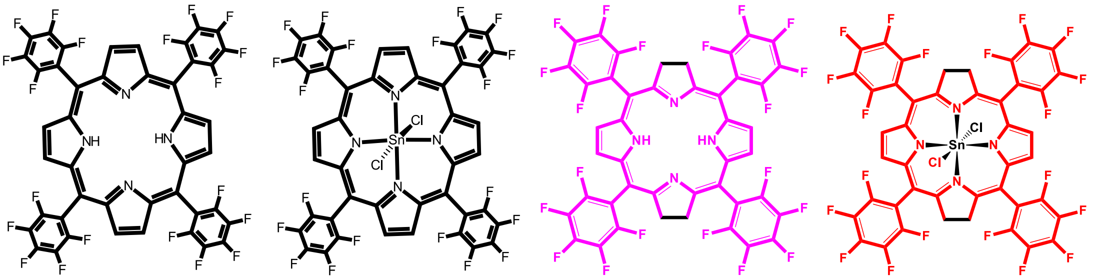

Figure 1. From left to right, free base tetra(pentafluorophenyl)porphyrin (**Penta**), Sn(IV) tetra(pentafluorophenyl)porphyrin (**SnPenta**), freebase bacteriochlorin (**PentaBChl**), and Sn(IV) tetra(pentafluorophenyl)bacteriochlorin (**SnPentaBChl**).

The key findings observed were that the pentafluorophenyl rings are strongly electron-withdrawing and play a large role in stabilising the BChl ligand, making it easier to synthesise tetra(pentafluorophenyl)BChls. Significantly lower IC_{50} values were obtained for the BChls relative to structurally analogous tetra(pentafluorophenyl)porphyrins, with the highest PDT activity being observed against MCF-7 breast cancer cells for **PentaBChl** and **SnPentaBChl**. This trend was also observed after the insertion of the metal into the core of the BChls. It was particularly noteworthy that high Log_{10} reduction values were obtained against Gram-(−) *E. coli* bacteria with free base and Sn(IV) tetra(pentafluorophenyl)BChls even in the absence of positively charged moieties, in a similar manner to what has been reported recently by Mack and coworkers for Sn(IV) tetraarylchlorins [6].

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Novel water-soluble chlorin photosensitizers for use in photoelectrochemistry and photodynamic therapy

Mahlatse Mokgaetjie Ledwaba[a], *Simone Bassini*[b,c], *Elise Daems*[b,c], *Earl Prinsloo*[d], *John Mack*[a], *Tebello Nyokong*[a] *and Karolien De Wael*[b,c]

Institute for Nanotechnology Innovation, Rhodes University, Makhanda 6140, South Africa, E-mail: j.mack@ru.ac.za. [b]Antwerp, engineering, photoelectrochemistry, and sensing (A-PECS), Department of Bioscience Engineering, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium. [c]NANOlight Center of Excellence, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium. [d]Biotechnology Innovation Centre, Rhodes University, Makhanda 6140.

Keywords: chlorins, singlet oxygen, photocurrent, photodynamic therapy

Chlorins have been explored for various applications, such as anticancer and antibacterial photodynamic therapy [1, 2]. However, their application in electroanalysis as photoresponsive materials is still at an early stage [3]. Water-soluble tetra-4-carboxyphenylchlorins have been synthesised and characterised (Figure 1a), including the free base dye (**H_2C**) and its *trans*-axially ligated Sn(IV) complex (**SnC**). **SnC** exhibited high solubility in PBS buffer and a high singlet oxygen ($^1O_2$) quantum yield of 0.70. The chlorins were used in photoelectrochemical studies, with higher photocurrents observed for **SnC** across most of the visible regions (Figure 1b). Photodynamic therapy activity studies against the MDA-MB-231 breast cancer cell line (Figure 1c-d), a triple-negative, aggressive, and invasive subtype used to model late-stage breast cancer, were conducted through 30 min irradiation with Thorlabs M625L3 (2.6 J.cm^{-2}) and Thorlabs M660L3 (3.0 J.cm^{-2}) LEDs. A favourable IC$_{50}$ value of 5.8 µM was obtained for **SnC**, while a higher value of 12.1 µM was observed for **H_2C**, demonstrating that water-soluble Sn(IV) tetraarylchlorin complexes merit further in-depth study for use as $^1O_2$ photosensitising dyes in biomedical applications.

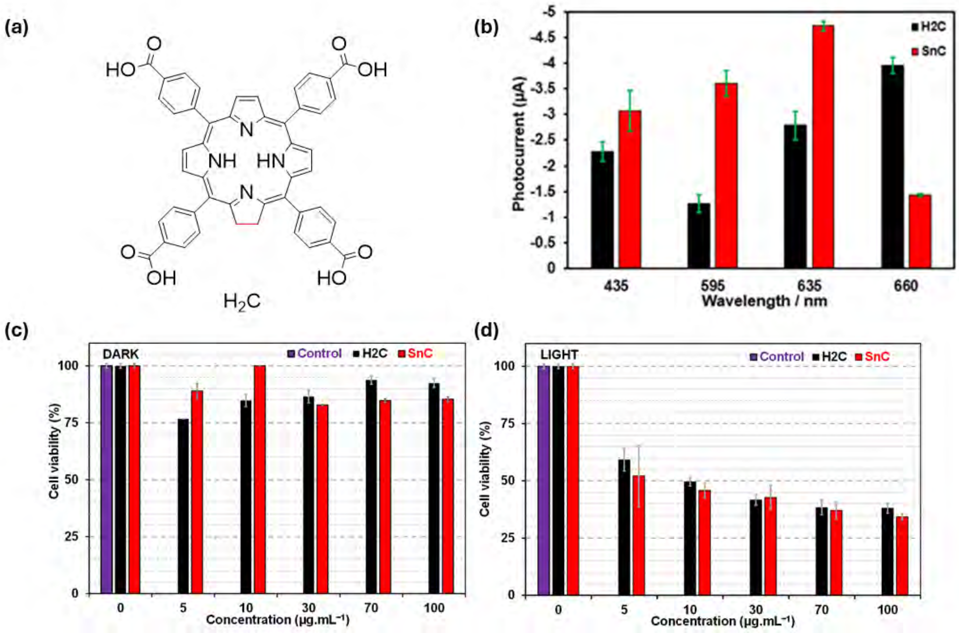

Figure 1. (a) Molecular structure of **H_2C**. (b) Comparison of the photocurrent generated by **H_2C** and **SnC** with LEDs at four different wavelengths. (c) Dark toxicity and (d) PDT activity graphs of **H_2C** and **SnC** against MDA-MB-231 cells at different concentrations.

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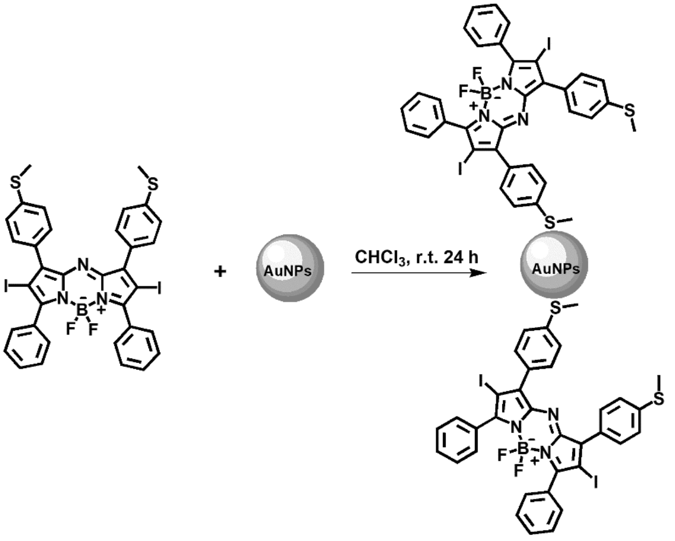
The photodynamic antimicrobial chemotherapy activities of azaBODIPY dyes and their gold nanoparticles conjugates

Temlandvo M. Magwaza, *Nthabeleng Molupe, Yolande I. Openda, John Mack and Tebello Nyokong*

Institute for Nanotechnology Innovation, Rhodes University, Makhanda 6140, South Africa, E-mail: j.mack@ru.ac.za (JM)

Keywords: azaBODIPY; gold nanoparticles; photophysicochemical properties; photodynamic antimicrobial chemotherapy

Boron dipyrromethene (BODIPY) dyes and their analogues, such as boron dipyrromethene (azaBODIPY), have been studied extensively for dye applications at the red end of the visible and near-infrared [1]. Their photophysicochemical properties can be modified through facile structural modification to enhance their suitability for biomedical photosensitizer dye applications [2]. The synthesis and photophysicochemical properties of two 2,6-diiodinated azaBODIPY dyes with thiomethylphenyl groups at the distal positions and phenyl (**1**) and naphthyl (**2**) rings at the proximal positions are reported. The dyes were conjugated to gold nanoparticles (**1**-AuNPs and **2**-AuNPs) to enhance their aqueous solubility for biomedical applications in a manner similar to what has been reported previously for porphyrin analogues [3].



1-AuNPs

Iodination at the 2,6-positions of the azaBODIPY core resulted in an enhancement of singlet oxygen generation, with singlet oxygen quantum yield (Φ_Δ) values of 0.82 and 0.55 obtained for **1** and **2**, respectively. The photodynamic antimicrobial chemotherapy (PACT) activities of the dyes were tested with a Thorlabs M660L4 light-emitting diode (LED) against *Staphylococcus aureus* after incubation at 5 µM. Conjugation to gold nanoparticles was found to significantly enhance the PACT activities against *Staphylococcus aureus*. Log$_{10}$ reduction values of 8.94 were obtained for **1**-AuNPs after 30 min irradiation (3.0 J.cm^{-2}) and **2**-AuNPs after 60 min (6.0 J.cm^{-2}).

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Impact of host-activator composition on UCNP photoluminescence

ML. Samsodien[a], ME. Meyer[b], T. Kroon[c], DR. Beukes[d], EM. Antunes[a]

[a]*Department of Chemistry, University of the Western Cape, Cape Town, South Africa, E-mail:* 3573207@myuwc.ac.za. [b]*Department of Biotechnology, University of the Western Cape, Cape Town, South Africa.* [c]*Department of Physics, University of the Free State, Cape Town, South Africa.* [d]*School of Pharmacy, University of the Western Cape, Cape Town, South Africa*

Keywords: upconversion nanoparticles, host lattice, sensitizer, activator

Upconversion nanoparticles (UCNPs) are nanoscale materials typically doped with lanthanide ions that have the remarkable ability to absorb multiple low-energy photons, most commonly in the near-infrared region, and emit a single photon of higher energy in the visible or ultraviolet region [1, 2]. They are composed primarily of three key components: a host lattice, sensitizer ions, and activator ions. The host lattice provides a stable crystalline framework with low phonon energy that facilitates efficient energy transfer; sensitizer ions absorb low-energy photons (often in the near-infrared range) and transfer the energy to activator ions, which then emit higher-energy photons in the visible or ultraviolet regions through an upconversion process. This unique ability to convert invisible infrared light into visible emissions have made UCNPs promising candidates in fields ranging from biomedicine and imaging to security and energy conversion [1, 2].

This study investigates how compositional variations in the host lattice ($NaYF_4$ vs. $NaScF_4$) and activator ions (Er vs. Ho) affect the luminescent properties of UCNPs. $NaYF_4$:Yb/Er, $NaYF_4$:Yb/Ho, and $NaScF_4$:Yb/Er nanoparticles were synthesized via a microwave solvothermal method. Structural information was obtained through X-ray diffraction as well as solid state ^{23}Na NMR, while particle sizes were confirmed through TEM images. The emissions of the nanoparticles once excited was determined through steady-state fluorescence spectroscopy. The sizes of the nanoparticles ranged from 10 to 200 nm with a cubic phase composition which was determined by the XRD pattern. The solid-state ^{23}Na NMR spectra displayed signals between 7 and –25 ppm and was particularly sensitive to the method of synthesis. The steady-state fluorescence spectroscopy showed that the $NaYF_4$:Yb/Er and $NaScF_4$:Yb/Er nanoparticles emitted three prominent bands corresponding to green and red emissions, with $NaScF_4$:Yb/Er uniquely exhibiting a strong emission at 810 nm. In contrast, $NaYF_4$:Yb/Ho nanoparticles demonstrated four emission bands across green, red, and near-infrared regions. These findings demonstrate that UCNP luminescence can be tuned by modifying host lattice and activator composition, highlighting their potential for multifunctional photonic applications.

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Design and characterization of norbornadiene-azobenzene hybrids for enhanced molecular solar thermal (MOST) energy storage

Buyane Ngubane and Dr Mpondi Molefe

Department of Chemistry, Rhodes University, Chemistry & Pharmacy Building, Makhanda, 6139, South Africa, E-mail: buyanengubane@gmail.com

Keywords: Molecular Solar Thermal (MOST), Norbornadiene, Azobenzene, Liquid Crystals, Diels-Alder reaction, Photoresponsive Molecules, Enegy Storage

Molecular Solar Thermal (MOST) systems offer a sustainable solution to global energy demands by capturing solar energy and storing it in the chemical bonds of reversible photoactive molecules. This study explores the synthesis and characterization of novel norbornadiene-based photoswitches functionalized with azobenzene moieties, known for their robust photoresponsive behaviour. The synthetic route involves thermal cracking of dicyclopentadiene to generate cyclopentadiene, followed by a Diels-Alder reaction with propiolic acid to form carboxylic acid-functionalized norbornadiene. This provides a versatile anchor point for attaching azobenzene derivatives with variable alkyl chain lengths, facilitating the formation of conjugated norbornadiene-azobenzene systems. The structural modifications are designed to enhance both photothermal energy storage capacity and thermal stability. A central aspect of this research is the evaluation of liquid crystallinity in these molecules, as mesophase behaviour is known to improve energy storage efficiency through better molecular alignment and packing. Differential Scanning Calorimetry (DSC) and Polarized Optical Microscopy (POM) are employed to identify and characterize liquid crystalline phases. The results aim to inform the development of next-generation MOST systems with optimized performance for both local and global solar energy applications.

The influence of chelating agents on the hydrodeoxygenation (HDO) performance of Cu promoted NiMo catalysts supported on alumina

[a] [a] - , and Zenixole R Tshentu

[a]Department of Chemistry, Nelson Mandela University, P.O. Box 77000, Gqeberha 6031, South Africa, E-mail: s225097001@mandela.ac.za.

Keywords: Hydrodeoxygenation, copper promoted catalysts, chelating agents in catalysts.

The rapid depletion of oil reserves and the environmental issues caused by the heavy reliance on fossil fuels throughout society's explosive growth have forced the world to find alternative sources of fuel. Fossil fuels can be satisfactorily replaced with biofuels such as biodiesel and bioethanol which are liquid fuels that are extensively used for transportation and industrial purposes. However, the processing of biocrudes is demanding due to the high concentration of oxygen-containing compounds. This study investigates the impact of chelating agents on the physicochemical properties of γ-Al_2O_3-supported NiMo and CuNiMo hydrodeoxygenation catalysts. The catalysts were prepared using co-impregnation with ethylenediaminetetraacetic acid, acetic acid, or citric acid as chelating agents [1]. Characterization techniques, including N_2 adsorption-desorption, XRD, UV-Vis DRS, FT-IR, SEM/EDX, and HRTEM, revealed that the presence of chelating agents prevented the formation of the crystalline β-$NiMoO_4$ phase and enhanced metal dispersion on the support [2]. Notably, citric acid promoted uniform copper, nickel, and molybdenum particle dispersion on alumina [3]. SC-XRD was used to explain why promoter metals such as Ni are known to sulfide later than Mo, since it was found embedded within a sphere of Mo-O. The maximal phenol conversion was observed for CuNiMo/γ-Al_2O_3 (46.1%) and NiMo/γ-Al_2O_3 catalyst had the lowest activity with the conversion of 42.1 % during hydrodeoxygenation at 300°C, 40 bar H_2 pressure, and 300 rpm agitation speed. The higher activity of CuNiMo/γ-Al_2O_3 catalyst was attributed to the presence of promoter Cu on the acidic alumina support that enhances dispersion of NiMo-S active phases [3,4]. The study provides insights into the role of chelating agents and promoter Cu in modifying the physicochemical properties of NiMo HDO catalysts.

, Rinae E Mugwena   Dele P Fapojuwo

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Non-proteinogenic amino acids based on quinoline scaffolds

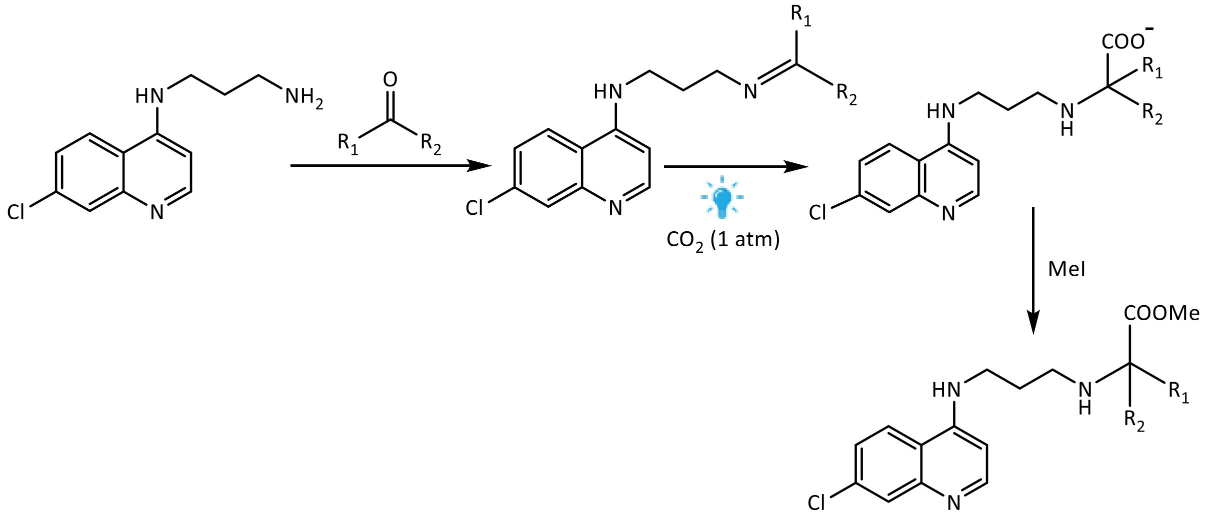
Relebohile Mbongo[a], *Gregory S. Smith*[a] *and Marwaan Rylands*[a]

[a]Department of Chemistry, University of Cape Town, Woolsack Drive, Rondebosch, 7701, South Africa, E-mail: mbnrel001@myuct.ac.za.

Keywords: amino acids, quinolines, anticancer

Non-proteinogenic amino acids (NPAAs) provide a broad chemical space for designing novel compounds with improved stability, selectivity, and functionality. Incorporating NPAAs into molecular frameworks can produce compounds with enhanced pharmacokinetics and bioactivity.[1] Quinoline scaffolds, a class of heterocyclic compounds, have garnered considerable attention in medicinal chemistry due to their diverse biological activities, particularly their anticancer properties.[2] Quinolines demonstrate antitumour effects through various mechanisms, including DNA intercalation, inhibition of topoisomerase, and modulation of signalling pathways.[3]

This presentation describes the design and synthesis of quinoline-based imines as key intermediates in developing novel NPAA analogues with potential anticancer activity. A modular synthetic approach was employed, and several quinoline-derived imines have been prepared and characterised using NMR spectroscopy, IR, and mass spectrometry. These intermediates are further transformed into target amino acid methyl esters for subsequent biological evaluation. This work lays the foundation for exploring structure–activity relationships of quinoline-based NPAAs in cancer therapy.



Scheme 1: General Synthetic Pathway

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Hydrogenation of Carbon dioxide (CO_2) to Methane Using $NiSe_2$-Based Catalysts Supported on Functionalized Carbon Materials

Lindokuhle Magagula[a], *Ella Linganiso*[b], *and Nosipho Moloto*[a,*]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Johannesburg, Wits, 2050, South Africa, E-mail: Nosipho.moloto@wits.ac.za. [b]Microscopy and Microanalysis Unit, University of the Witwatersrand, Private Bag 3, Johannesburg, Wits, 2050, South Africa

Keywords:. CO_2 Hydrogenation, $NiSe_2$ Catalyst, Methanation, Carbon Materials, Renewable Energy, Waste-to-Economy

The continuous rise in atmospheric CO_2 levels, driven by industrialization and fossil fuel consumption, demands urgent strategies for carbon mitigation. CO_2 hydrogenation to methane presents a promising route for carbon recycling and clean energy production [1]. In this study, we report the synthesis and characterization of nickel selenide ($NiSe_2$)-based catalysts for the selective methanation of CO_2. $NiSe_2$ was chosen due to its optimal carbon monoxide (*CO) adsorption energy and resistance to CO poisoning, which enhances catalytic stability and CH_4 selectivity at low temperatures (250–300 °C) [2] X-ray diffraction (XRD) confirmed the formation of crystalline, phase-pure cubic $NiSe_2$ (PDF- **00-041-1495)**, with three strong peaks at $2\theta = 29.8$, 33.4, and 36.7° corresponding to the (2 0 0), (2 1 0), and (2 1 1), crystal planes, shown in Fig. 1 (d). Transmission electron microscopy (TEM) revealed agglomerated, pollen-like $NiSe_2$ particles (Fig. 1 (c)), while scanning electron microscopy (SEM) showed a rough, porous morphology favorable for gas-phase catalysis (Fig. 1 (d)). These structural features suggest an increased density of active sites and efficient gas diffusion pathways. To further enhance performance, $NiSe_2$ will be supported on functionalized graphitic carbon nitride ($g\text{-}C_3N_4$) to introduce surface vacancies and promote electron mobility. Alternatively, nitrogen-doped carbon nanotubes (N-CNTS) will be used for their high surface area and conductivity. This work contributes to sustainable CO_2 conversion strategies while promoting waste-to-economy applications through the development of carbon-supported catalysts. Fig. 1a demonstrates the graphical abstract.

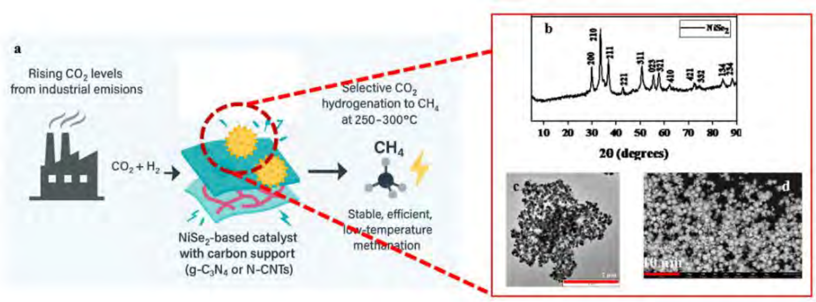

Figure 1. (a) Graphical abstract depicting the concept of selective CO_2 hydrogenation to CH_4 using a $NiSe_2$-based catalyst with carbon supports ($g\text{-}C_3N_4$ or N-CNTs). (b) XRD pattern confirming the phase-pure cubic structure of $NiSe_2$. (c) TEM image showing agglomerated, pollen-like $NiSe_2$ particles. (d) SEM image highlighting the rough and porous morphology of the $NiSe_2$ catalyst, favourable for gas-phase catalysis.

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Multifunctional molecular architectures for enhanced solar thermal energy storage

NF Molefe, Bongeka Ndwandwe, Buyane Ngubane and Khanya Mafentile

Department of Chemistry, Rhodes University, Chemistry & Pharmacy Building Makhanda, 6139 PO Box 94, Makhanda, 6140, South Africa, E-mail: m.molefe@ru.ac.za

Keywords: Molecular Solar Thermal (MOST), Norbornadiene, Azobenzene, Liquid Crystals, Fluorination, Perylene, Energy Storage, Photothermal Materials

The growing global demand for clean and decentralized energy solutions has intensified the search for advanced materials capable of efficiently capturing, storing, and releasing solar energy. Molecular Solar Thermal (MOST) systems offer a unique approach to solar energy storage by using reversible photoactive molecules to absorb sunlight and convert it into chemical energy, which can be released as heat on demand [1].

This research presents a multi-pronged strategy to enhance MOST performance by developing and characterizing three distinct classes of functional molecular systems. First, we synthesize norbornadiene-azobenzene (NBD-Azo) hybrids, combining two robust photoswitch motifs to improve thermal stability and photoconversion efficiency. The design enables conjugation between components and provides modularity through alkyl chain and azobenzene substitution.

Second, we explore a series of fluorinated azobenzene-based liquid crystalline compounds, where structural tuning via alkyl chain length and fluorine substitution is used to optimize mesophase behaviour, light absorption, and energy storage density. Characterization by DSC, POM, UV-Vis, and DFT reveals that these systems display tunable red-shifted absorption and enhanced photothermal properties.

Third, we investigate the role of perylene derivatives as performance enhancers in MOST systems due to their photocatalytic behaviour, favourable energy transfer dynamics, and charge-separation abilities. Together, these systems represent a modular platform for next-generation MOST materials with tailored properties for efficiency, scalability, and integration into real-world solar energy applications.

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Synthesis and structural characterization of O^N^O-donor Zn and Mn complexes as catalysts for the production and depolymerization of PLAs

Asanda Ngwenya, Mnqobi Zikode, Stephen. O. Ojwach

School of Chemistry and Physics, University of KwaZulu-Natal, Pietermaritzburg Campus, Private Bag X01, Pietermaritzburg 3209, South Africa. Email: 221009466@stu.ukzn.ac.za

Keywords: catalysts, polymerization, depolymerization, poly(lactides)

The mass production of synthetic plastics remains one of the largest contributors to environmental pollution. Particularly, the prevalence of single-use plastics (SUPs) continues to undermine recycling efforts employed to combat their ubiquity.[1] Approximately 76% of these conventional, petroleum-based plastics end up in landfills or discharged into the natural environment.[2] This has prompted research devoted to the production of bio-based polymers, derived from renewable resources. PLAs have emerged as promising ecofriendly substitutes to fossil-based plastics, owing to their biodegradability, bio-assimability, eco-compatibility and renewability. [3] Herein, we report the syntheses of mononuclear and multinuclear Zn and Mn complexes supported by imino-phenol Schiff base ligands. Structural characterization of the complexes using spectroscopic techniques, elemental analyses and single crystal X-ray crystallography revealed complexes with diverse coordination modes. All complexes proved to be highly performing multi-purpose catalysts in the ring-opening polymerization of rac-lactide to produce PLA and the degradation of PLA to give the green solvent, methyl lactate (Fig. 1).

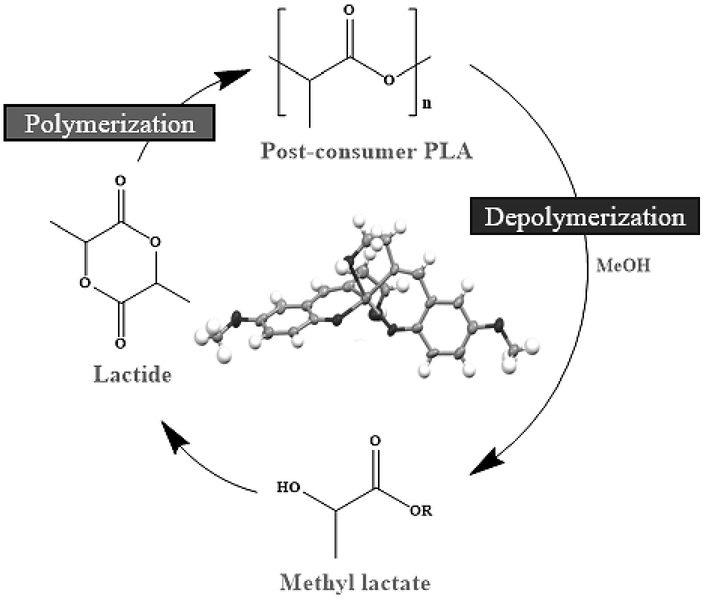

Fig. 1: Zn/Mn catalyzed production and depolymerization of poly(lactides).

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An approach to artificial photosynthesis: A molecular coordination of ligands focusing on p-Bromophenyl arsonic acid

Rika van Dyk, *Richard Betz, and Eric Hosten*

Department of Chemistry, Nelson Mandela University, University Way, Summerstrand, Gqeberha, 6019, South Africa, E-mail: s224232975@mandela.ac.za

Keywords: Artificial photosynthesis, spiroarsoranes, p-bromophenyl arsonic acid, main group chemistry, pentacoordination.

Organoarsenic chemistry has been studied for centuries, and various properties, including aromaticity, frontier molecular orbitals, and inversion energies, have been predicted by computational methods. Concerns, however, were raised about the synthesis procedures associated with these compounds, restricting all experimental investigations. The latter led to the evolution of NIT methods that ensure the safe production of functional organoarsenic compounds [1]. This study focuses on synthesizing and characterizing the starting material: p-Bromophenyl arsonic acid as well as spirocyclic structures, both derived from arsenic and characterizing them in the solid state and in solution, together with baseline spectroscopic data, as there is a lack of data (Figure 1). Knowing whether simple neutral compounds could extend the coordination sphere from five to six would be interesting [2].

The project aims to construct a system that can host three reaction centers, enabling the artificial photosynthesis steps within the respective centers. An additional objective includes the coordination of carbon dioxide to the Arsenic center, ultimately yielding oxygen and carbohydrates. Spiroarsoranes assume one of two geometries: trigonal bipyramidal or square pyramidal. Saturated, bulky chelating agents on the metal center increase the thermal stability of the complex, whilst small aliphatic diols decrease the thermal stability. Smaller substituents were noted to prefer an SP geometry, whilst larger groups favoured TBP geometries. It is hypothesized that the molecules with SP geometry have a great affinity for a sixth bonding partner since steric hindrance will have little impact on this coordination type. However, this could also lead to instability of the attached carbon molecule.

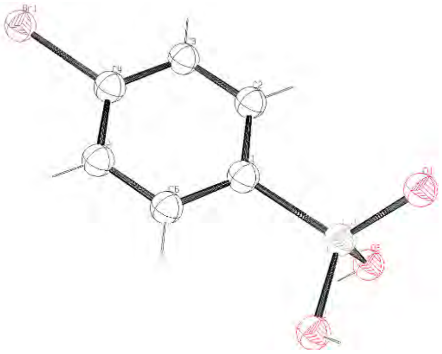

Figure 1: ORTEP representation of the p-Bromophenyl arsonic acid that function as the starting material for the spiroarsorane complexes.[3]

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Exploiting hybrid metal-based strategies to target *M. abscessus*

Lesedi Lale[a], *Monique Williams*[b] *and Gregory Smith*[a]

[a]Department of Chemistry, University of Cape Town, Rondebosch, Cape Town, 7700, South Africa, E-mail: llxles002@myuct.ac.za. [b]Department of Molecular and Cell Biology, University of Cape Town, Rondebosch, Cape Town, 7700, South Africa

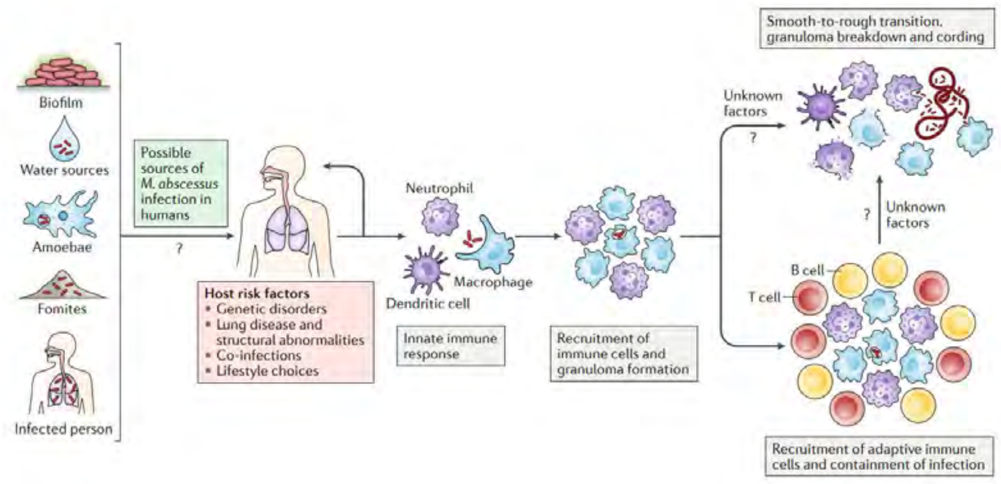
Keywords: benzimidazole, triazole, ferrocene, molecular hybridization

M. abscessus is a rapidly growing mycobacteria that was first reported by Moore and Frerichs in 1953.[1] *M. abscessus* has an infection process like *M. tuberculosis*, but there is limited knowledge on the actual routes of transmission. Infections can remain dormant in a patient for years longer than a decade without showing symptoms and later be found in patients' granulomas during lung biopsy.[2]

Reports have indicated that standard antituberculous agents are ineffective towards *M. abscessus* due to rising resistance.[3] There is a need to develop novel antimicrobial agents that will overcome the bacterial resistance. Benzimidazoles are privileged heterocyclic biological entities that can be used to develop new antimicrobial agents due to their similarity with purine. Another strategy explored recently to counter the resistance is that of molecular hybridization through combining known drugs with privileged pharmacophoric scaffolds.[3]

Metal-based drugs show distinct mechanisms of action relative to conventional organic antibiotics.[4] In particular, iron complexes of 1,2,4-triazole Schiff bases have also been shown to indicate an increased antimicrobial activity against several gram-positive and gram-negative bacteria relative to the individual ligands.[4]

This preliminary study focuses on the synthesis of two benzimidazole-pyrazine molecular hybrids, one comprising of a phenyl linker and the other in which a triazole is incorporated and including a bioisosteric ferrocenyl metallofragment. The minimum inhibitory concentration of all the target hybrid compounds is evaluated against *M. abscessus* strains.



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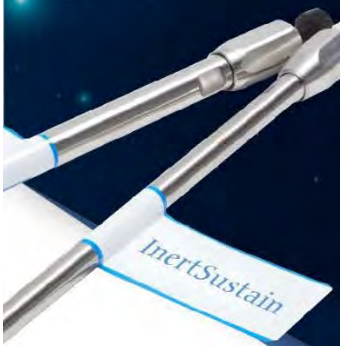

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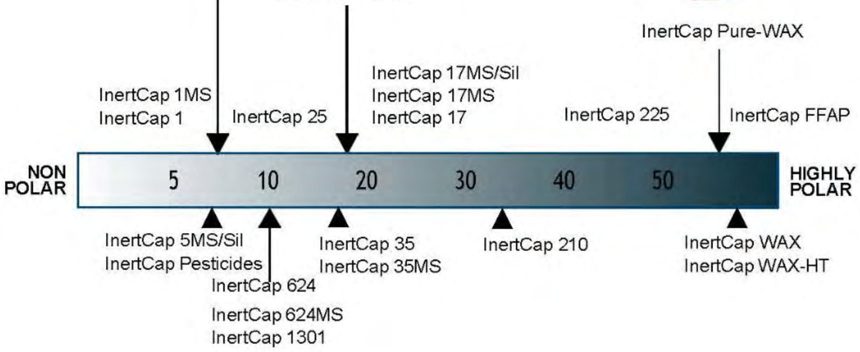

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Design and optimization of fluorinated azobenzene-based liquid crystalline systems for molecular solar thermal energy storage

K. Mafentile, NF. Molefe, B. Ndwandwe

Department of Chemistry, Rhodes University, Grahamstown, 6140, South Africa, Email: g22m3607@campus.ru.ac.za

Keywords: Molecular Solar Thermal (MOST), Azobenzene, Liquid Crystals, Fluorine Substitution, Photothermal Energy Storage, Photoconversion, Energy Materials

As global energy demands rise and energy insecurity intensifies particularly in regions burdened by frequent load-shedding there is an urgent need for reliable, scalable, and renewable energy storage solutions. Molecular Solar Thermal (MOST) systems represent a promising class of materials capable of capturing solar energy and storing it in the form of high energy photoisomers, with heat release on demand. This research focuses on the molecular engineering of azobenzene derivatives designed to function as efficient MOST candidates, with an emphasis on inducing and optimizing liquid crystalline (LC) behaviour to improve energy density and system organization.

A series of azobenzene-based compounds were synthesized, incorporating alkyl side chains of varying lengths to modulate molecular packing, phase behaviour, and thermal stability. To enhance photochemical efficiency and broaden light absorption, electron-withdrawing fluorine substituents were strategically introduced into the aromatic core. Comprehensive characterization was conducted using spectroscopic (NMR, FTIR, UV-Vis), thermal (TGA, DSC), structural (XRD), and microscopic (POM) techniques, along with Density Functional Theory (DFT) calculations to predict theoretical energy storage capabilities.

Initial results indicate that fluorinated azobenzene derivatives exhibit favourable red-shifted absorption, improved photostability, and enhanced mesophase formation. Compounds with longer alkyl chains demonstrated superior thermal energy storage potential, attributable to improved LC order and higher enthalpy of phase transitions [1]. These findings support the development of structurally tunable MOST materials tailored for solar energy harvesting in low-resource environments [2].

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Synthesis and characterization of Co, Ni, and Cu sulphide nanoparticles using dithiocarbamate complexes as single source precursors for the electrochemical reduction of nitrates to ammonia

Thabiso Sibambo[ab]; *Nosipho Moloto*[ab]; *Izak Kotze*[ab]; *Poslet Shumbula*[ab*]

[a] Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Wits, 2050, South Africa
[b] DSI/NRF Centre of Excellence in Strong Materials, University of the Witwatersrand, Braamfontein 2050, South Africa

Keywords: single-source precursor, selectivity, efficiency

The electrochemical nitrate reduction reaction has recently gained interest as remedial alternative of the energy intensive Haber-Bosch process. This project aims to address both nitrate contamination and green ammonia production through the development and optimization of HDA-capped Co, Ni, and Cu sulphide nanoparticles as catalysts for the NO_3^-RR. Dithiocarbamate complexes were employed as single-source precursors for the synthesis of the nanoparticles through the colloidal hot injection method. These metal chalcogenides were analysed using X-ray diffraction, Transmission electron microscopy, scanning electron microscopy, UV-Vis spectroscopy, Energy dispersive X-ray microscopy, and Fourier-Transform Infrared microscopy to determine structural formation, phase purity, crystallinity, size and their morphology. The electrochemical performance of the metal chalcogenides was evaluated for the reduction of nitrates to ammonia. Electrochemical measurements such as linear sweep voltammetry and chronoamperometry were employed to assess the activity, selectivity and efficiency of the nanoparticles, and these parameters varied based on the type of catalyst being used. This study demonstrates the efficiency of metal chalcogenides as electro-catalysts for effective nitrate to ammonia conversion, providing a sustainable approach to ammonia synthesis and wastewater treatment.

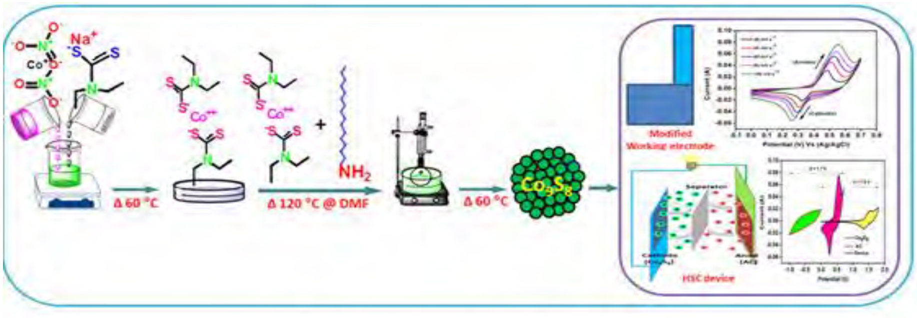

Fig. 1. Schematic diagram of Co_9S_8 nanoparticles.

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Investigation of NiN nanoparticles as electrocatalysts in nitrate reduction to ammonia

Ts'epo Tumeli, Juanita van Wyk and Nosipho Moloto

School of Chemistry, University of the Witwatersrand, Private Bag X3, Johannesburg, 2050, South Africa
richard.tumeli1@wits.ac.za

Keywords: Bis(pyrrolaldiminato) nickel (II) complexes, NiN nanoparticles, electroreduction, nitrate, ammonia

The electrocatalytic reduction of nitrate to ammonia (e-NO_3RR) offers a sustainable alternative to the Haber–Bosch process. The process can be used to recover ammonia from nitrate-polluted water using renewable electricity and the ammonia can be reused in fertilizers and chemicals/fuel, **Figure 1 a** [1,2]. This approach turns environmental waste into valuable resources. A wide variety of electrocatalysts have been investigated, including monometals (e.g., Ru, Pd, Cu), alloys (e.g., CuNi), metal oxides (e.g., Cu_2O, Co_3O_4, TiO_2), and metal nitrides (e.g., Ni_3N), each offering different advantages and limitations [2]. Noble metals exhibit outstanding activity and selectivity but are prohibitively expensive and not scalable. Transition metal-based nanomaterials, especially nitrides, have emerged as promising alternatives due to their high conductivity, tunable surface chemistry, and earth-abundant nature. Among these, nickel-based systems are of particular interest, offering a balance of catalytic efficiency and cost-effectiveness. Further engineering of nanomaterials through precursor control, defect modulation, and phase tuning continues to drive improvements in selectivity and Faradaic efficiency.

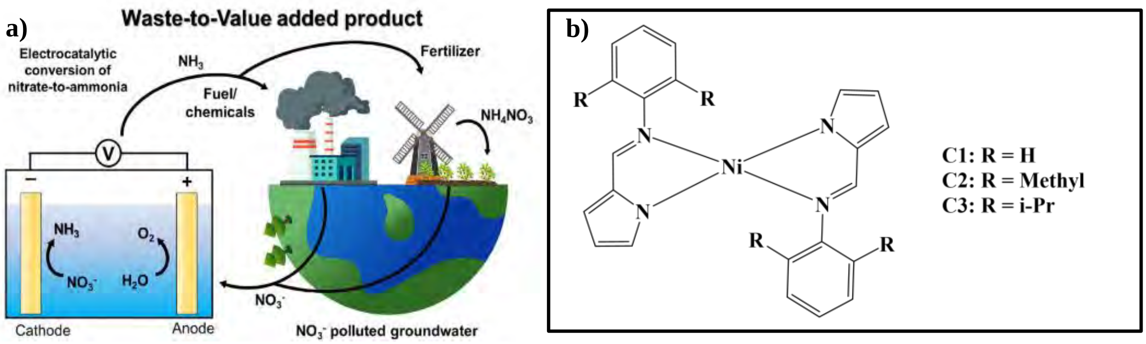

Figure 1: *a) Electrocatalysis system for Nitrate reduction to Ammonium (e-NO_3RR) [2] b) bis(pyrrolaldiminato) nickel (II) complexes.*

In this study, we report the use of bis(pyrrolaldiminato) nickel (II) metal complexes, **Figure 1 b**, as single-source precursors for the synthesis of nickel nitride (NiN) nanoparticles via thermal decomposition using various capping agents (TOP, HAD, oleylamine) under inert conditions. The influence of ligand architecture, reaction temperature, and precursor concentration on particle morphology and crystallinity will be studied [3]. The resulting NiN nanoparticles will be investigated as electrocatalysts for nitrate reduction to ammonia in an effort to develop scalable and cost-effective nanocatalysts for sustainable ammonia production [4].

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The effect of salicylic acid-derived passivators on room temperature synthesised $CsSnBr_3$ perovskites

Thato Makgaka[a], Arthur Moya[a], Grace Ngubeni[a], Pierre Mubiayi[a], Nosipho Moloto[a,b]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg 2050, South Africa. Email: 543294@students.wits.ac.za [b]DSI-NEDBANK SARChI in Energy Materials, University of the Witwatersrand, Johannesburg 2050, South Africa. Email: Nosipho.moloto@wits.ac.za

Keywords: Perovskite, salicylic acid, solar cell

In 2022, South Africa had more than 80% of it's energy production through coal and other non-renewable energy resources [1]. With the amount of renewable energy resources available in the country such as wind, water, and the solar energy, the opportunity is there to utilize it for renewable energy production. As such, energy production through solar energy presents an opportunity to meet the energy demands of the country. The dominant production of solar energy is through the use of silicon solar panels. While these are a staple in a lot of houses around the world, the installation cost is expensive [2]. As such, cheaper material may be required to make solar energy more affordable to homes. Perovskites have garnered great attention due to the low cost of material, a higher efficiency potential, and the potential use of flexible materials vs silicon wafers [3]. This study aims to investigate the properties of tin perovskites synthesized at room temperature using salicylic acid and its derivatives as capping agents and furthermore evaluate the percent conversion efficiency of the solar cells. The results show that synthesis using salicylic acid and its derivatives as capping agents allows for the formation of tin perovskites at room temperature without the use of any harmful solvents or the need for a neutral atmosphere, showing the possibility of expanding the synthesis to other perovskite material. It showed stability of more than a week, and a similar performance during that duration. As such, the method shows a promising way of synthesizing stable all inorganic tin perovskites in ambient air for solar cells applications.

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Synthesis of conductive polymer/onion-like carbon composites gas sensor for the detection of ammonia at room temperature

Ketshepile Baabua[a], Manoko-Maubane NKadimeng[a] Siziwe Gqoba[b], Cebisa Linganiso[b]

[a]Research Centre for Synthesis and Catalysis, School of Chemistry, University of Witwatersrand, Private Bag 3, Braamfontein 2050, Johannesburg, South Africa.γ [b]Centre for Carbon-nano Science Research, University of Witwatersrand, South Africa. Email: Manoko.Maubane@wits.ac.za

Keywords: Onion-like carbons (OLCs), Conductive polymers, Polymer/OLC composites, Ammonia Sensing, Gas Sensor materials, Carbon nanomaterials

Ammonia (NH_3) is mostly employed in industrial, agricultural, and medical applications, but its harmful effects and instability demand the development of effective, inexpensive detection devices. This study investigates the synthesis and use of conductive polymer/onion-like carbon (OLC) composites as gas sensors for ammonia detection at room temperature. OLCs were produced using an environmentally friendly, inexpensive flame pyrolysis method from waste cooking oil, providing an environmentally sustainable pathway to advanced carbon compounds. Three conductive polymers, such as polyaniline (PANI), polypyrrole (PPy), and polythiophene (PTH), were synthesized and combined with OLCs to determine their gas-sensing performance. The synthesized materials were characterized using BET, TEM, SEM, XRD, FTIR, TGA, and Raman to evaluate their morphological, structural, and surface properties. This work aims to determine the most active polymer-OLC combination with promising potential for room-temperature ammonia gas detection.

Periodic trends of tungsten boride, carbide, nitride, oxide, phosphide, sulfide catalysts for hydrodeoxygenation of biocrude oil

Ndiphiwe Mahlaka, *Tendai Dembaremba, Dele Fapojuwo and Zenixole Tshentu*

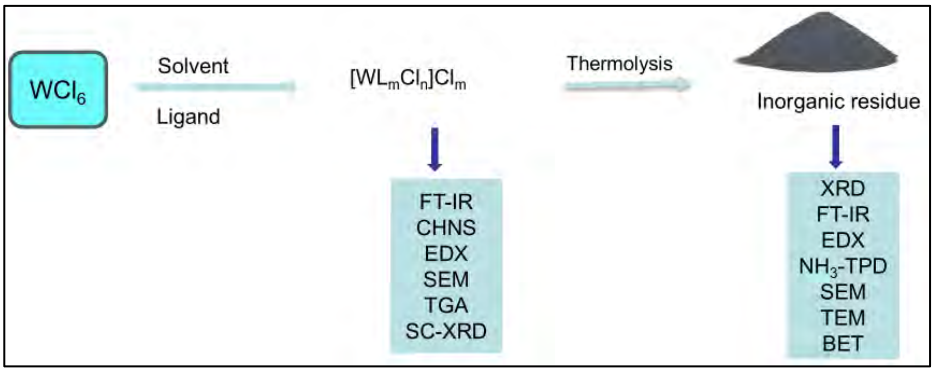
Department of Chemistry, Nelson Mandela University, Gqeberha, 6031, South Africa, E-mail: s219481490@mandela.ac.za

Keywords: Biofuel, hydrodeoxygenation, coordination complex, thermolysis, catalyst.

Biofuel contains high levels of oxygen and water, lowering its calorific value when compared of petroleum oil and high viscosity and low pH value making the oil undesirable for ignition engines. Conventional hydrotreating catalysts are designed for normal crude oil that does not contain the high oxygen content, and this leads to catalyst deactivation through dealumination, coking and sintering. Transition metal boride, carbides, nitrides, and phosphide exhibit noble metal-like characteristics and are now being investigated as alternative cost-effective candidates for hydrotreatment. However, synthesis of these catalysts involves metal oxide precursor, harmful and flammable gases, such as CH_4, NH_3, PH_3, and H_2S at high temperature. Other drawbacks of using solid-gas method are low-purity, poor size and morphology of the products.

There is a lack of periodic trends for the various active metals and their counter elements in HDO catalysis. As such, we sought to lay groundworks for screening the activities and selectivies for tungsten borides, carbides, nitrides, oxides, phosphides, and sulfides catalysts. The preliminary work in this project has therefore focused on developing a new strategy for synthesis of these catalysts from metal complexes that can then be calcined under more ambient conditions to obtain these catalysts.

FT-IR, CHNS, SEM-EDX, and TGA-DSC were used to confirm the successful synthesis of tris(ethylenediamine)tungsten(VI) chloride, bis(diphenylphosphine)tungsten(VI) chloride and bis(ethanedithiol)tungsten(VI) chloride complexes. Thermolysis of the synthesized complexes at a specific temperature produced various phases including simple tungsten, tungsten-rich and nonmetal-rich materials. Thermal degradation results in loss on organic bonds such as C-H between and carbon nonmetal bonds such as C-N, C-P, and C-S from the ligand. These materials will be characterized further using XRD, TEM, NH_3-TPD, and BET and their hydrodeoxygenation activity will be evaluated using model compound such as phenol in a fixed-bed reactor.



Scheme 1: A schematic for the synthesis tungsten borides, carbides, nitrides, oxides, phosphides, and sulfides for determining the trends in hydrodeoxygenation catalysis.

Investigating Bis(salicylidiminato) nickel (II) complexes as precursors for the preparation of NiO nanoparticles

Phathutshedzo Makhumisane, Ts'epo Tumeli, Juanita van Wyk and Nosipho Moloto

School of Chemistry, University of the Witwatersrand, Private Bag X3, PO Wits, 2050, South Africa, E-mail: 2878580@students.wits.ac.za

Keywords: Ammonia (NH_3), nitrate (NO_3^-), electrochemical nitrate reduction, salicylaldimine ligands, nickel complexes, NiO nanoparticles

Ammonia (NH_3) is a zero-carbon molecule that plays a significant role for sustaining life on Earth, serving as a key component in the chemical industry, agriculture, medicine and a renewable hydrogen carrier [1]. Human activities are releasing nitrate (NO_3^-) into land and water systems, causing environmental pollution. This not only threatens human health and living creatures but also disrupts the nitrogen cycle because of the large amounts involved [2]. Electrochemical nitrate reduction (e-NO_3RR) offers societal benefits by converting nitrate pollutants into valuable ammonia, effectively transforming waste into wealth [3]. This work focuses on investigating bis(salicylidiminato) nickel (II) complexes for the preparation of NiO nanoparticles using the single source precursor approach. In this study the ligand architecture is varied to determine if there is an influence of substituent group on the NiO nanoparticles produced. The nickel complexes were obtained by reacting nickel acetate tetrahydrate with three different *N*-(aryl)salicylaldimine ligands in a 2:1 mole ratio. All ligands and nickel complexes were characterized using spectroscopy techniques such as NMR, FT-IR and UV-Vis as well as elemental analysis. The colloidal method was used for the synthesis of NiO nanoparticles due to its flexibility since it allows variation of reaction parameters. The crystalline structure, morphology, shape and size of the synthesized NiO prepared are investigated using, powder X-ray diffraction (PXRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM).

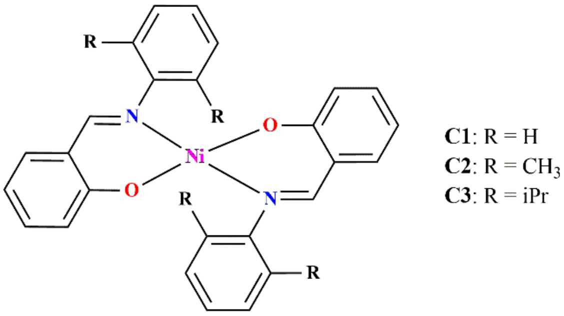


Figure 1: Structures of bis(salicylidiminato) nickel(II) complexes investigated in this study

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Elucidating the physiochemical properties of KOH-activated onion-like carbons for application in DSSCs

Keneilwe Khoza[a], *Grace Ngubeni*[a] *and Manoko Maubane-Nkadimeng*[a,b]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Johannesburg, 2050, South Africa, E-mail: 2326658@students.wits.ac.za. [b]Microscopy and Microanalysis Unit, University of the Witwatersrand, Private Bag 3, Johannesburg, 2050, South Africa

Keywords: OLC, KOH activation, counter electrode, dye-sensitized solar cells

The adverse impacts of non-renewable energy sources have made research into renewable substitutes increasingly critical. Dye-sensitized solar cells (DSSCs) are among the most studied 3rd generation solar cells owing to their facile fabrication, flexibility, and competitive efficiency [1]. These utilize platinum (Pt) as the state-of-the-art catalyst for the counter electrode (CE) due to its outstanding electrocatalytic properties. However, Pt's high cost and low abundance hinder their widespread application [1–2]. Carbonaceous materials have shown immense potential to replace Pt since they are abundant, stable, and display good electrical conductivity [3]. Nonetheless, studies show that when applied in DSSCs, the power conversion efficiency of carbon materials remains lower than that of Pt [3]. As such, there is a need to further develop and optimize nanocarbons as electrocatalysts. This study approaches this by improving the electrochemical performance of onion-like carbons (OLCs) through the introduction of porosity and disorder to the material. OLCs synthesized from the flame-pyrolysis of waste engine-oil were subjected to chemical activation using KOH in different OLC:KOH ratios (1:1–1:5). The XRD data confirmed the presence of amorphous C(002) and C(100) planes in the pristine OLCs (P-OLCs) and activated OLCs (A-OLCs). Raman spectroscopy showed the D/G area ratio to increase with activation ratio. The BET surface area analysis highlighted that the activation drastically increased the surface area of the material, with A-OLC 1:4 exhibiting the highest surface area (1635 m^2/g). Moreover, electrochemical studies in the iodide/triiodide electrolyte revealed the reduction peak current density of the P-OLC to be 3.6 mA/cm^2 while that of A-OLC 1:4 was increased to 7.2 mA/cm^2. Therefore, these findings underscore the potential of activated OLCs derived from waste as sustainable alternative CEs in DSSCs.

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Strategies for incorporating Ni into zeolite pore channels to obtain catalysts with enhanced hydrogen spillover activity

Maano Mukwevho[a], *Dele P Fapojuwo*[a], *Tendai O Dembaremba*[a] *and Zenixole R Tshentu*[a]

[a]Department of Chemistry, Nelson Mandela University, P.O. Box 77000, Gqeberha 6031, South Africa, E-mail: s225097001@mandela.ac.za

Keywords: Zeolite catalysts, nickel phosphine complexes, liquified fuel gas.

Global warming remains a hot topic, and strong efforts are being made to reduce CO_2 emissions and CO_2 capture and utilization is a promising prospect [1]. Carbon capture technologies are being coupled with carbon utilization approaches that include production of fuels that will replace traditional fossil fuels. One such fuel is liquified fuel gas (LFG), an equivalent of liquified petroleum gas (LPG). LFG is a considerably environmentally friendly substitute for LPG and will provide the much-needed relief of the grid in South African household and for industrial needs while contributing to carbon offsetting efforts. While successes in converting CO_2 to dimethyl ether (DME) have been achieved, converting DME into LFG remains a challenge where efforts to increase conversion rates by increasing reaction temperature and pressure using the common zeolite catalysts results in poor selectivity for the desired propane and butane [2]. We proposed incorporation of nickel into zeolite cavities to improve hydrogen spillover and enhance conversion rates with good selectivity using more favourable reactions conditions. However, nickel is difficult to incorporate into the zeolite cavities due to their hydrophobic properties. We therefore developed a strategy of driving nickel complexes based on phosphine ligands (**Figure 1**) into zeolite channels using solvents of low dielectric constants. Nickel loading of at least 1 wt.% were achieved as confirmed by ICP analysis. HR-TEM and SEM confirmed good distribution and nano-scale particle size distribution of Ni in beta zeolite. Successful calcination and reduction to obtain Ni nanoparticles in the cavities were achieved with guidance from TG and TPR studies. The study developed a new series of catalysts that are promising for the DME to LFG conversion step.

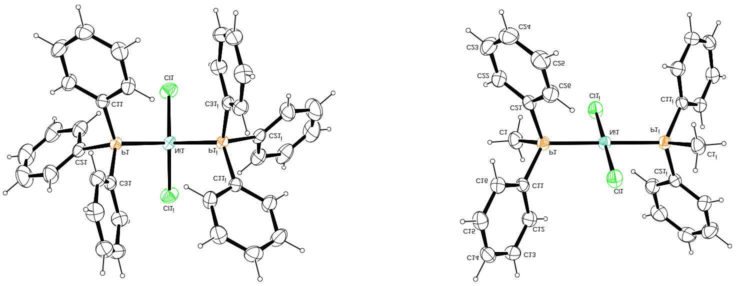

Figure 1. Nickel complexes used for incorporation of nickel into the zeolite channels.

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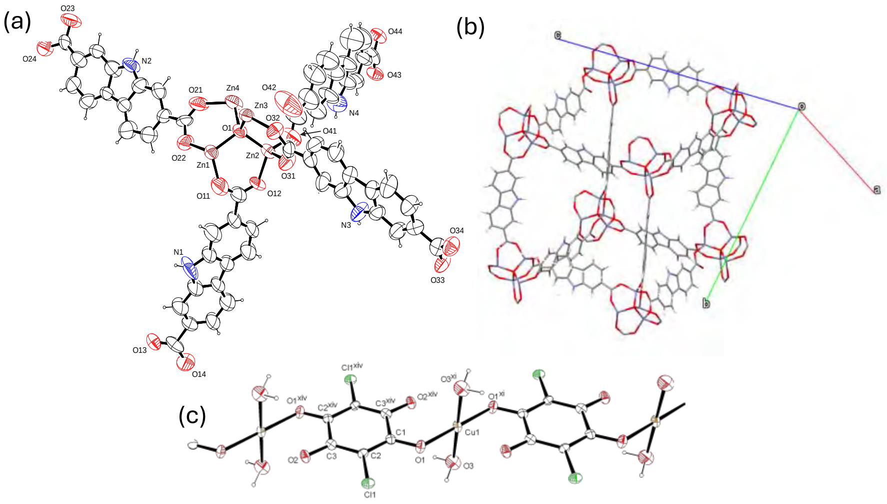
Nanoarchitecture of coordination polymers for selective adsorption of nitrogen containing compounds in hydrocarbon feeds

Tendai O. Dembaremba[a], *Adeniyi S. Ogunlaja*[b] *and Zenixole R. Tshentu*[a]

[a]Department of Chemistry, Nelson Mandela University, Gqeberha, Port Elizabeth, 6031, South Africa, E-mail: TendaiD@mandela.ac.za

Keywords: Coordination polymers, metal organic frameworks, adsorptive denitrogenation, nano-architecture.

Pyrolysis coupled with carbon capture technologies is considered a techno-economically viable alternative to produce sustainable aviation fuels.[1] The subject is gaining traction recently since it has been accepted that it will take time to replace certain petroleum derived transportation fuels such as aviation and shipping fuels by greener alternatives.[1-3] Likewise, adsorptive denitrogenation (ADN) of liquid hydrocarbon fuels, especially bio-oils, has gained attention due to its importance in ridding nitrogen containing compounds (NCCs) that have negative effects in the storage, processing and use of these fuels.[2,3] Primitive materials such as aluminosilicates and activated carbons, and advanced materials such as functionalized polymers and metal organic frameworks have been extensively investigated in that regard.[1,3] The complex nature of hydrocarbons feeds necessitates maximizing unique interactions that distinguish nitrogen containing compounds from the rest of compounds in the fuel matrix to achieve high selectivity that these materials are struggling with.[3] As such, this work sought to develop strategies for (i) adopting multiple interactive forces that work in synergy, and (ii) focus on coordinatively unsaturated metal sites that are highly selective for NCCs while minimizing all the other general types of interactions. Both strategies yielded positive outcomes, with the latter emerging as a novel adsorptive approach with much higher adsorption capacity (841.07 mg quinoline per g adsorbent) and selectivity. In this work, the inorganic chemistry considerations leading to the development and application of these coordination polymers obtained through nano-architecture approaches are unpackaged. The work is also accompanied by comprehensive studies in confirming chemisorption of quinoline on dehydrated copper chloranilic acid coordination polymer [Cu(CA)] using spectroscopic techniques, chemisorption and DFT studies.



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Carbon dots and tungsten disulfide hybrid for the detection of meat spoilage

Botle Molefi [a], *Nosipho Moloto*[a], *Manoko Maubane-Nkadimeng*[ab] *and Siziwe Gqoba* [a]

[a] School of Chemistry (Humphrey Rakes Building), University of the Witwatersrand, Private Bag 3, Wits, 2050 South Africa, E-mail: 1512312@students.wits.ac.za. [b]Microscopy and Microanalysis Unit, University of the Witwatersrand, Private Bag 3, Johannesburg, 2050, South Africa

Keywords: Carbon dots, Tungsten disulfide, Chemiresistive sensor

Ammonia (NH_3) is a key volatile biomarker for protein degradation during meat spoilage[1]. This project develops a novel, low-cost chemiresistive sensor based on a hybrid nanocomposite of carbon dots (CDs) synthesized from glucose and tungsten disulfide (WS_2) nanosheets for rapid, sensitive NH_3 detection. Glucose-derived CDs, synthesized via a facile microwave assisted method, provide abundant surface functional groups enhancing NH_3 adsorption, while WS_2 nanosheets offer excellent electrical conductivity and a high surface area platform. The CDs/WS_2 hybrid was characterized using FTIR, Raman spectroscopy, XRD, HTEM, UV- Vis and PL, confirming successful synthesis.

The chemiresistive sensor operates at room temperature, exhibiting a significant and reversible increase in electrical resistance upon exposure to NH_3 gas. This response is attributed to the electron-donating nature of adsorbed NH_3 molecules modulating the carrier concentration in the p-type WS_2, amplified by the synergistic interaction with the CDs. The sensor demonstrated high sensitivity towards NH_3, achieving a low detection limit, a rapid response time of XXX seconds, and excellent selectivity against common meat spoilage interferents such as Hydrogen sulfide and ethanol.

This glucose-CDs/WS_2 chemiresistive sensor offers a promising, scalable solution for real-time, non-destructive monitoring of meat freshness, with potential for integration into smart packaging systems to enhance food safety and reduce waste.

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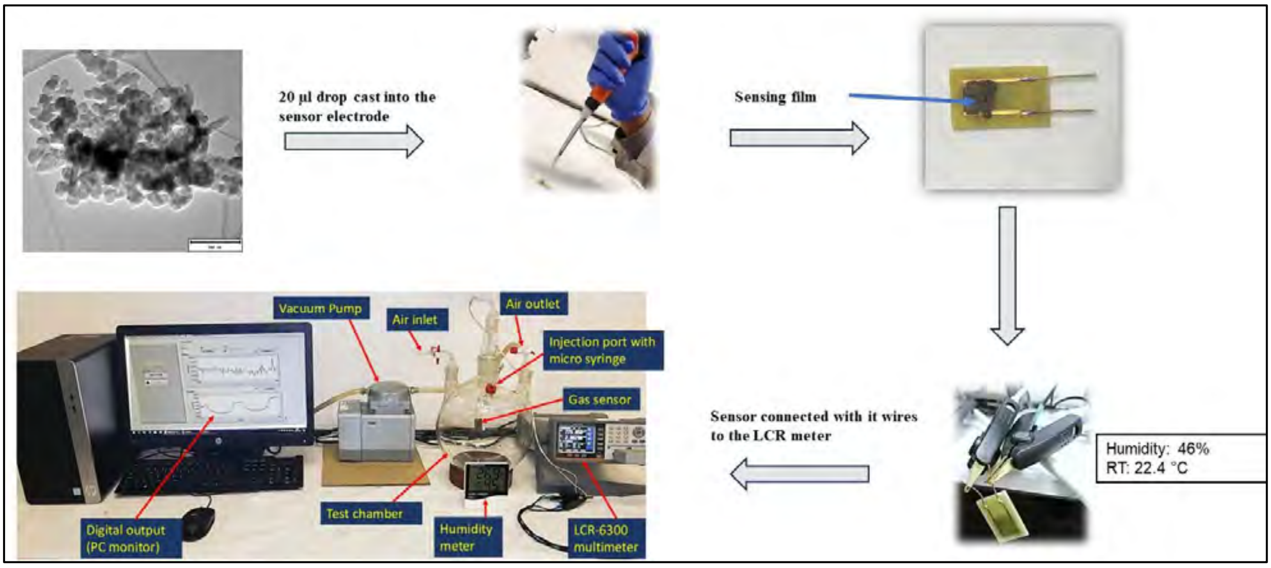
Evaluating the room temperature sensing properties of PANI/WS_2/OLCs composite towards ammonia vapour

Zamangwane Hlatshwayo[a], Zukiswa Mnqokoyi[a], Manoko Maubane-Nkadimeng[b], Lerato Machogo-Phao[c] and Siziwe Gqoba[a]

[a]Molecular Science Institute, School of Chemistry, University of the Witwatersrand, Braamfontein, 2050, South Africa, E-mail: 2107045@students.wits.ac.za. [b]Microscopy and Microanalysis Unit, University of the Witwatersrand, Braamfontein, 2050, South Africa, [c]Mintek, Randburg, 2190, South Africa

Keywords: room temperature, ammonia, OLCs, gas sensing, chemiresistive sensors

Air pollution associated with commercial industries is a concern in the environment. Ammonia gas is consumed and released often in the fertilizer industry, textile industry for the synthesis of dye, in the refrigerator as a coolant and also in the pesticide industry. Continual exposure may lead to health-related issues in humans and affect our ecosystem [1]. Polymers such as polyaniline can be fabricated as gas sensors for the detection of ammonia at room temperature. To address the harmful effects of ammonia, we synthesized a PANI/WS_2/OLC composite ex-situ for the detection of ammonia vapour. XRD and EDS confirmed the formation of the composite. The fabricated sensor material was then evaluated at room temperature towards ammonia vapour. The sensor showed good selectivity towards ammonia vapour compared to other volatile organic compounds. This was attributed to the synergistic effects created when these materials meet at the heterojunctions.



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Ethanol-enabled pyridyl-pyrazole manganese (I) catalysis: Sustainable transfer hydrogenation of nitriles with amine boranes

Tshegofatso Molapo[a], *Andrew J. Swarts*[a]

[a]Swarts Research Group, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa.

Keywords: manganese catalysis, transfer hydrogenation, pyridyl-pyrazole ligands, amine boranes, sustainable chemistry

Manganese catalysts offer sustainable alternatives to precious metals for nitrile transfer hydrogenation (TH), yet solvent selection remains critical. While isopropanol dominates TH for its hydrogen-donor capacity and recent Mn catalysis utilised diethyl ether [1], ethanol's potential is unexplored despite superior green metrics. Pyridyl-pyrazole Mn(I) complexes were evaluated for nitrile TH using dimethylamine borane (DMAB). Conversions (^{19}F NMR/GC-MS) and selectivity were assessed at 65–80°C. Kinetic studies probed mechanistic pathways. Under optimised conditions (3 mol% catalyst, 3 equiv. DMAB), ethanol achieved 93.4–94.8% conversion, rivalling isopropanol (96.6 – 97.1 %) while offering enhanced sustainability (low cost, toxicity). Catalyst-free controls confirmed ethanol's negligible background conversion (0% vs. 16.6 % for isopropanol). Ethanol's efficiency, unprecedented in TH catalysis, enables near-quantitative reductions without noble metals. This work establishes pyridyl-pyrazole Mn complexes as efficient catalysts for nitrile hydrogenation in ethanol - a breakthrough solvent for sustainable transformations. The ligand design overcomes limitations of commonly used phosphine systems and challenges of isopropanol/ether dependence.

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The development of Pd-loaded SAPO-13 chabazite zeolite catalysts for the conversion of DME to green liquified fuel gas (gLFG)

Luzuko Mbumbulwana[a], Fapojuwo Dele[a], Tendai Dembaremba[a] and Zenixole Tshentu[a]

[a]Department of Chemistry, Nelson Mandela University, Summerstrand, Gqeberha, 6001, South Africa, E-mail: mbumbulwanaluzuko@gmail.com

Keywords: liquified fuel gas, catalyst fabrication

The increase in global warming and CO_2 emissions has led to novel methods of capturing and utilizing CO_2 from the atmosphere for the production of more environmentally friendly non-petroleum-based energy fuels such as green liquified fuel gas (gLFG). However, bottlenecks are still present in the experimental optimization of this system, especially in obtaining the desired hydrogenated ratio of propane/butane selectivity. Hence, this work has focused on a catalyst design strategy of fabricating transition metal-incorporated zeolite catalyst towards enhanced catalytic performance and selectivity towards C_3/C_4 (LFG). The improvements involve the slight acid dealumination of microporous CHA-13 zeolite using 1 M HNO_3 under moderate reflux to increase porosity, acidity and hydrophobicity for appropriate shape product selectivity. Thereafter, to enhance hydrogenation, Pd-loading on dealuminated CHA-13 at Pd loading of 0.1- 0.5 wt% was conducted under controlled nitrogen reflux using dichlorido*bis*(dimethylphenylphosphine)palladium(II) complex, followed by reduction. Characterization of the catalysts was conducted by FT-IR, UV-Vis spectra to identify the present functional groups, while the ICP confirmed the Pd-loading wt% and zeolite ratio. Moreover, TEM is used to confirm the catalyst morphology (**Figure 1**) and SEM-EDS for Pd distribution [1-3].

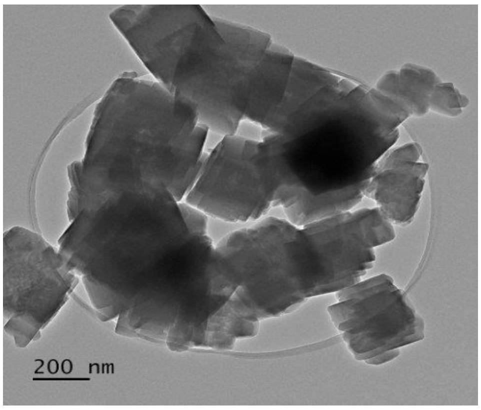

Figure 1. TEM micrograph of modified SAPO-13.

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Biomolecular affinities and cytotoxicity of copper(I) and silver(I) phosphine–pyridinyl complexes against Caco-2 and Caski cell lines

Adesola A. Adeleke[a,c], *Miche D. Meyer*[b], *Nicole R.S. Sibuyi*[b,c], *Martin O. Onani*[b], *Bernard Omondi**[c]

[a]Department of Chemical Sciences, Olabisi Onabanjo University, Ago-Iwoye, PMB 2001 Nigeria. [b]DSI/Mintek Nanotechnology Innovation Centre, Biolabels Research Node, Department of Biotechnology, University of the Western Cape, Private Bag X17, Bellville, 7535, South Africa. [c]School of Agriculture and Science, Discipline of Chemistry, University of KwaZulu-Natal, Private Bag X54001, Westville 4000, South Africa.

Keywords: Pyridinyl Schiff bases, triphenylphosphine, CT-DNA intercalation, Cytotoxicity

A series of three copper (I) and three silver (I) complexes with the general formula [M L$(PPh_3)_2$]NO_3, (M = Cu for complexes **1 – 3** and Ag for complexes **4 – 6**) were synthesized by reacting copper(I) or silver(I) -nitrate and triphenylphosphine with the bidentate ligands, (*E*)-1- (pyridin-2-yl)-*N*-(*o*-tolyl)methanimine **L1**, (*E*)-*N*-isopropyl-1-(pyridine-2-yl)methanimine **L2**, or (*E*)-*N*-(2,6-dimethylphenyl)-1-(pyridine-2-yl)methanimine **L3**. The structures of these complexes were elucidated using a combination of NMR spectroscopy, FTIR, UV-visible, mass spectrometry, elemental analysis, and single-crystal X-ray diffraction. Structural analysis revealed that the Schiff bases coordinate to the metal centres in a bidentate fashion, with triphenylphosphine occupying the remaining coordination sites in complexes **1**, **2**, and **5**. In contrast, in complexes **3**, **4**, and **6**, one coordination site is occupied by a nitrate anion instead of triphenylphosphine. All six complexes exhibit a distorted tetrahedral geometry around the metal centre, as confirmed by τ4 values ranging from 0.54 to 0.87.

Binding studies with calf-thymus DNA (CT-DNA) demonstrated that complexes **1** – **6** interact via intercalation, with complex **5** exhibiting the highest binding constant. Furthermore, all complexes showed strong binding affinity toward bovine serum albumin (BSA). Cytotoxicity studies revealed significant cytotoxicity of complexes **1** – **6** against human colon adenocarcinoma (Caco-2) and human cervical epidermoid carcinoma (Caski) cell lines.

Practical access to novel azomethines via mechanochemically driven Schiff-base reactions

Simnikiwe Nogqala[a], *Rosalyn Klein*[a] *and Xavier Siwe-Noundou*[b]

[a] Department of Chemistry, Rhodes University, Drosty Rd, Makhanda, 6139, E-mail: snogqala97@gmail.com, [b]Sefako Makgatho Health Sciences University, Pretoria 0204, South Africa

Keywords: Mechanochemical imine synthesis, Silica sulfuric acid (SSA) catalyst, solvent-free mechanochemistry

Mechanochemical synthesis has emerged as a sustainable and efficient alternative to conventional solution-phase protocols in organic chemistry [1]. Herein, we introduce a convenient, affordable, and solvent-free mechanochemically assisted protocol for the preparation of imine (azomethine) derivatives, using sulfuric acid adsorbed on silica gel (silica sulfuric acid, SSA) as a recyclable solid acid catalyst in a planetary ball mill.

Under controlled planetary ball-milling conditions, equimolar mixtures of amines and carbonyl containing reagents were ground with SSA at ambient temperature, without any solvent. For comparison, analogous runs were performed using acetic acid as the catalyst under identical milling conditions. The conventional reflux method (in solution with SSA) was employed in parallel to benchmark performance. Catalyst recycling was evaluated by recovering SSA after reaction, washing, and reusing it for a total of six successive runs, with yields recorded at each cycle.

The mechanochemical SSA protocol yielded up to 83%, markedly exceeding the maximum of 68% obtained under conventional reflux conditions. In contrast, acetic acid under mechanochemical conditions delivered only 63% maximum yield, underscoring the enhanced acidity and catalytic efficiency of solid-supported sulfuric acid under grinding. The SSA catalyst retained high activity through six cycles, showing only minimal decline in yield, highlighting its robustness and reuse potential. These findings align with the known mixing and thermal effects of ball milling that favour condensation equilibria under solvent-free conditions [2].

This novel SSA-ball-mill method offers a superior, eco-friendly, and cost-effective route to imine derivatives compared to traditional reflux. Key advantages include higher yields, solid acid catalysis, solvent elimination, and efficient catalyst recyclability. The protocol thus provides a compelling alternative for both academic and industrial synthesis of azomethine compounds, advancing the fields of green chemistry and mechanochemical organic synthesis.

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The synthesis and characterization of $CsCuBr_3$ perovskites for the degradation of pharmaceutical waste in water

Grace Chota[a] *Grace N. Ngubeni, Pierre K. Mubiayi*

[a]Department of Chemistry, University of the Witwatersrand, 1 Jan Smuts Avenue, Johannesburg, Braamfontein, 2001, South Africa, E-mail: 2153197@students.wits.ac.za

Keywords: Pharmaceutical contaminants, perovskites, photocatalysis

The increasing contamination of water bodies by pharmaceutical contaminants such as antibiotics and painkillers has raised concerns about their long-term effects on humans and aquatic life. This has prompted the emergence of efficient and environmentally friendly remediation technologies to mitigate current challenges such as low efficiency, toxicity or reliance on UV light. This project aims to synthesize sustainable, lead-free $CsCuBr_3$ halide perovskites for the photodegradation of pharmaceutical contaminants in water.

Copper is both chemically stable, cost-effective, low in toxicity and earth-abundant compared to conventional lead. A colloidal synthesis method has been employed to synthesize $CsCuBr_3$ perovskites which will be characterized by structural, morphological and optical techniques including X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM) or Transmission Electron Microscopy (TEM), Ultraviolet-Visible Spectroscopy (UV-Vis) and Photoluminescence (PL) spectroscopy. Preliminary results have confirmed the synthesis of Cs_2CuBr_4 and $Cs_2Cu_3Br_5$ phases with an absorption edge range of 250- 320 nm and peak emission of 419 nm, however, further synthesis, characterization and optimization is yet to be undertaken.

Photocatalytic performance testing is planned to assess the efficiency of the perovskite to degrade selected pharmaceutical contaminants under visible light exposure. This research not only offers a safer alternative to lead-based photocatalysts, but also supports sustainable development goal 6, promoting access to clean water and sustainable environmental practices and expanding on the knowledge of perovskites in terms of their potential for scalability.

Nickel(II) Schiff base complexes as electrode materials for enhanced energy storage in asymmetric supercapacitor coin cells

Ibrahim Wazirit[a], *Tunde L. Yusuf*[b], *Kaushik Mallick*[a] *and Sarit K. Ghosh*[a]

[a]Department of Chemical Sciences, University of Johannesburg, P.O. Box 524, Auckland Park 2006, South Africa
[b]Department of Chemistry, Faculty of Natural and Agricultural Science, University of Pretoria, Private Bag X20, Hatfield 0028, Pretoria, South Africa, E-mail: triumph2236@gmail.com

Keywords: Ni-complex, Schiff base, dielectric polarization, supercapacitor electrode, asymmetric coin cell

In this study, three different nickel (II)-based Schiff base ligand complexes, derived from condensation of 2-hydroxybenzaldehyde with 2-bromo-4-chloroaniline (C1), 2-bromo-4-methylaniline (C2), and 2-iodo-4-nitroaniline (C3), were synthesized using a one-pot *in-situ* reaction strategy without isolating the ligands. The synthesized complexes were characterized using standard spectroscopic techniques, with the solid-state structure for C1 and C2 were determined through single-crystal X-ray diffraction analysis. The Schiff base-derived complexes, C1, C2, and C3 systems, were fabricated as an electrode material, and their electrochemical performance was evaluated in a 2 M KOH solution. The cyclic voltammetry analysis confirmed their pseudo-capacitive behaviour, as evidenced by the redox peaks. Among the three electrodes (C1, C2 and C3) the 2-iodo-4-nitroaniline based electrode (C3) exhibited superior electrochemical charge storage capability and along with higher polarizability in dielectric constant. At 1 A.g^{-1}, the C3 electrode delivered maximum specific capacitance value of ~ 330 F.g^{-1}while maintaining excellent cycling stability of ~ 96.5 %after 2000 charge-discharge cycles at 5 A.g^{-1} An asymmetric (AC//C3) super capacitor coin cell operated under the potential of 1.6 V, delivered a specific capacity of ~ 98.3 C.g^{-1} (~ 27.3 mAh.g^{-1}) at 0.5 A.g^{-1}. The device demonstrated a high energy density of ~ 21.8 Wh.kg^{-1} with power density of ~ 378.3 W.kg^{-1} at 0.5 A.g^{-1}, reaching a maximum power density of ~ 1089 W.kg^{-1} at 4.0 A.g^{-1}. Furthermore, two-coin cells connected in series can generated a voltage of ~ 2.91 V, sufficient to power a red LED, demonstrating its potential for practical energy storage applications.

Simple ruthenium catalysts for the formic acid dehydrogenation: Insights into catalytic strategies and mechanistic insights

Pamela. S. Moyo[a], *and Andrew. J. Swart*

[a]School of Chemistry, University of Witwatersrand Johannesburg, Jorissen St, Braamfontein, Johannesburg, 2017, South Africa. Email: pamela.moyo@wits.ac.za.

Keywords: Homogenous, ruthenium, hydrogen storage, formic acid dehydrogenation

Hydrogen (H_2) plays a significant role as a renewable and clean energy source in mitigating the impacts of climate change and the energy crisis associated with fossil fuels.[1] Researchers aim to find an economical source and methods with enhanced properties (i.e., high production rate, lower cost, safe and more available) for H_2 production and storage. Hydrogen has a high specific energy, high density and can be used for various applications. Most popular hydrogen storage materials are organic compounds, so-called liquid hydrogen carriers (LOHCs).[2] Formic acid (HCOOH, FA) is one of the most promising liquid organic hydrogen carriers as it features high volumetric energy density, low toxicity and is liquid at room temperature.[3] Both homogenous and heterogenous based-catalysts have been explored for the formic dehydrogenation process under mild conditions with homogeneous metal-based complexes constitute the state-of-the-art catalysts.[4-5] This work focuses on the synthesize and characterization of ruthenium(II) complexes bearing bipyridine-based ligands for the FA dehydrogenation. The simple ruthenium catalysts have been synthesized and characterized using various spectroscopic and analytical techniques.

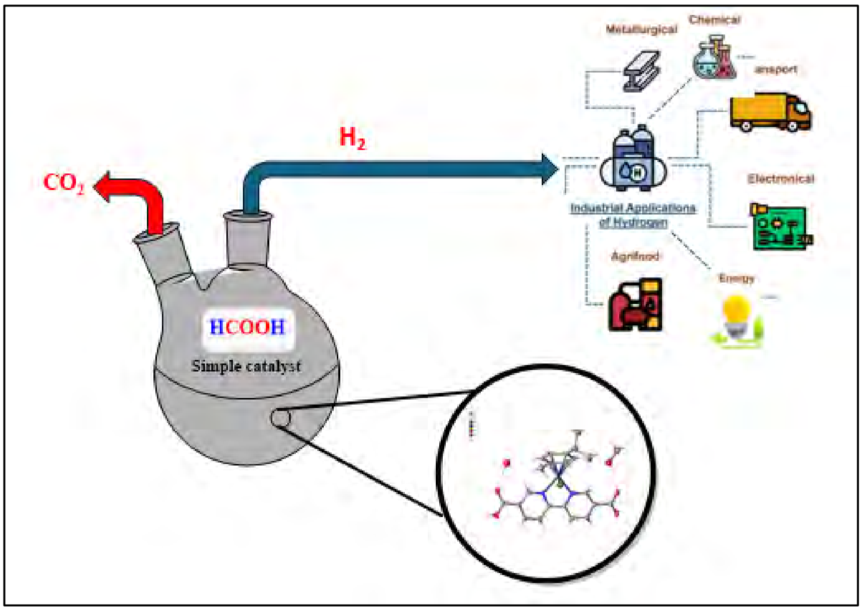

Figure 1. Graphical abstract

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Zeolitic imidazolate framework integrated by gold nanoclusters for selective desulphurisation of fuel oil

Ms. TK Magunda, Dr. Otun K, Prof Nomvamo Mketo

University of South Africa, Department of Chemistry

Keywords: ZIFs, desulphurisation, selectivity

The selective removal of sulfur compounds from fuel oil remains a critical challenge in the pursuit of clean and safe energy for the user, the environment, and the engines. [1] In this study, we report the synthesis and application of a novel composite material—gold nanoclusters integrated into a Zeolitic Imidazolate Framework (ZIF)—for efficient desulphurisation. The hybrid system leverages the high surface area and tunable porosity of ZIFs alongside the catalytic activity of gold nanoclusters [2] to target refractory sulfur species such as dibenzothiophene. Characterization techniques, including XRD, TEM, and BET analysis, confirmed successful integration and structural stability of the composite. Adsorptive desulphurisation performance [3] was carried out and evaluated under mild conditions, demonstrating enhanced selectivity and removal efficiency compared to conventional adsorbents. The synergistic interaction between the ZIF matrix and gold nanoclusters facilitates improved adsorption kinetics and regeneration capability. These findings highlight the potential of ZIF–Au nanocluster composites as a promising platform for sustainable fuel purification technologies [4,5].

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Interfacial engineering of $CsMBr_3$ (M = Mn, Fe, Ni) thin films for enhanced charge transfer in perovskite-sensitized solar cells

Simphiwe Ngwenya[a], *Pierre Mubiayi*[a] *and Nosipho Moloto*[a]

[a]Department of Chemistry, University of the Witwatersrand, School of Chemistry, Private Bag 3, Wits 2050, South Africa. E-mail: 1597591@students.wits.ac.za . Kalenga.Mubiayi@wits.ac.za ; Nosipho.Moloto@wits.ac.za

Keywords: All-inorganic, interfacial, thin-films, charge transfer

All-inorganic halide perovskites are emerging as promising light absorbers for stable and efficient solar energy conversion; however, interfacial charge losses remain a critical bottleneck to device performance [1,2]. In this study, we investigate the effect of B-site cation substitution in $CsMBr_3$ (where, M = Mn, Fe, or Ni) on the optical, morphological, and interfacial charge-transfer properties of perovskite-sensitized solar cells. UV–Vis absorption spectroscopy revealed composition-dependent band-edge positions with steep absorption onsets, indicative of low urbach energies. Atomic force microscopy (AFM) and scanning electron microscopy (SEM) confirmed continuous coverage of the perovskite films on TiO_2/ITO, with AFM-derived thicknesses of 518 nm ($CsMnBr_3$), 352 nm ($CsFeBr_3$), and 577 nm ($CsNiBr_3$), and root-mean-square roughness values of 90.3 nm, 54.6 nm, and 75.7 nm, respectively. The relatively high roughness compared to total film thickness indicates pronounced grain-to-grain height variations, consistent with the polycrystalline and granular morphologies observed in SEM. Steady-state photoluminescence (PL) measurements showed pronounced quenching for films on TiO_2 relative to the corresponding powders, consistent with enhanced electron injection into TiO_2. The combination of favorable morphology, suitable thickness, and strong PL quenching in $CsMnBr_3$ and $CsNiBr_3$ suggests improved perovskite/TiO_2 interfacial coupling and reduced recombination losses [3]. These findings demonstrate that B-site cation engineering in $CsMBr_3$ enables concurrent optimization of film morphology, thickness, and interfacial electron transfer, providing a viable pathway toward stable, high-performance all-inorganic perovskite photovoltaics.

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Conformational isomers of cinnamoyl quinoline hybrids as corrosion inhibitors for zinc and aluminium in hydrochloric acid

K.B Moloto, L.C Murulana, M.V Bvumbi and G.M Masuku

Department of Chemistry, Faculty of Science, Engineering and Agriculture, University of Venda, Private Bag X5050, Thohoyandou, 0950, South Africa, E-mail: 21002552@univen.ac.za

Keywords: corrosion, inhibitor, adsorption, cinnamoyl quinoline hybrids

Corrosion causes the deterioration of metals, making them unattractive and weaker [1]. Various corrosion mitigations have been explored over the years. The current best mitigation is the use of corrosion inhibitors [2]. This study evaluates the corrosion inhibition potential of conformational isomers of cinnamoyl–quinoline hybrids for zinc and aluminium in 1 M HCl at 30-60 °C. Cinnamoyl quinoline hybrids were synthesized and characterized by Nuclear Magnetic Resonance (NMR) and Infrared (IR). Electrochemical impedance spectroscopy (EIS), potentiodynamic polarisation (PDP), and gravimetric analysis techniques were utilized to assess the corrosion inhibition properties of the studied compounds. Fourier transform infrared spectroscopy (FTIR) was utilized to learn more about the functional groups that appeared or disappeared during the adsorption/desorption of the inhibitor molecules on the metal. The amount of metal content in solutions will be determined using atomic absorption spectroscopy (AAS). The surface morphology of the uninhibited and inhibited processes will be examined using energy dispersive spectroscopy (EDS) in conjunction with scanning electron microscopy (SEM). The results from carbon and proton NMR showed that all the protons and carbons obtained from the synthesized structures were well accounted for, showing that cinnamoyl quinoline hybrids were successfully synthesized. The gravimetric analysis results obtained, revealed that aluminium corrodes faster than zinc in hydrochloric acid. They also showed that temperature is directly proportional to corrosion rate. The findings suggest cinnamoyl–quinoline hybrids hold promise as effective corrosion inhibitors in acidic media.

Fig 1: Metal before and after experiencing corrosion [3].

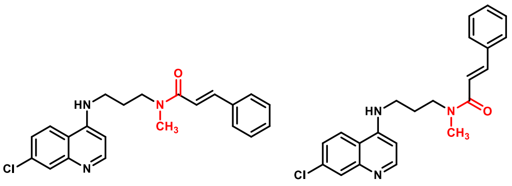

Fig 2: Rotameric forms of the hybrids.

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Sustainable ceramic membranes functionalized with Ag-doped ZnO for enhanced photodegradation of methyl orange

KA. Malebadi[a,b], *NH. Seheri*[a,b], *DC. Onwudiwe*[a,b*]

[a]*Material Science Innovation and Modelling (MaSIM) Research Focus Area, Faculty of Natural and Agricultural Sciences, North-West University, Mafikeng Campus, Private Bag X2046, Mmabatho, 2735, South Africa*
[b]*Department of Chemistry, School of Physical and Chemical Sciences, Faculty of Natural and Agricultural Sciences, North-West University, Mafikeng Campus, Private Bag X2046, Mmabatho 2735, South Africa*
**Corresponding author's email: Damian.Onwudiwe@nwu.ac.za.*

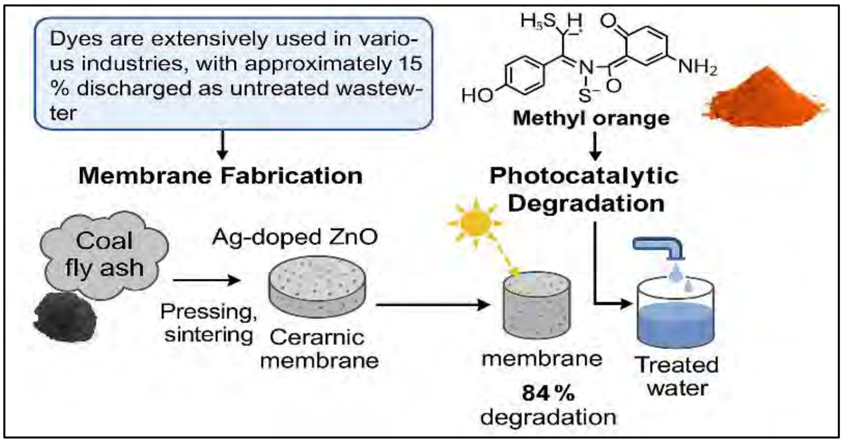
Keywords: doped Metal oxide; Photocatalytic membrane; Methyl orange degradation; Water treatment; Sustainable Development Goal 6 (SDG 6)

Dyes are extensively used in various industries, with approximately 15% discharged as untreated wastewater. Due to their complex aromatic structures, high solubility, and low biodegradability, these untreated dyes such as methyl orange (MO), pose significant risks to humans and aquatic lives. MO, an anionic azo dye, is toxic, carcinogenic, and teratogenic, disrupting aquatic ecosystems by blocking sunlight penetration, and depleting dissolved oxygen levels. Conventional water treatment methods often fail to fully degrade MO, necessitating advanced remediation approaches.

This study presents a novel Ag-doped ZnO functionalized coal fly ash-derived ceramic membrane fabricated via a combined pressing and sintering method. The intrinsic properties of the functionalized membranes were characterized and their chemical and physical properties such as chemical stability, mechanical stability, water absorption, and porosity were established. The shape, crystallinity, thermal characteristics, and functional groups present were also determined using SEM, XRD, TGA, and FTIR studies, respectively.

The optimal membrane functionalized with 10% Ag-doped ZnO and sintered at 1000 °C exhibited an excellent thermal/chemical stability and suitable porosity for ultrafiltration. Photocatalytic degradation study of methyl orange (MO), used as a model pollutant, showed an optimum efficiency of 84% achieved within 120 min of visible light irradiation. Moreso, the functionalized membrane was found to be stable with 80% degradation efficiency obtained after 5 consecutive cycles of reusability study, showing negligible loss of efficiency.

This work provides a practical foundation for scalable photocatalytic membranes in industrial wastewater treatment, supporting sustainable development goal 6. Further scale-up and their utilization in real industrial applications will validate their robustness for environmental remediation.



Synthesis and characterisation of polyaniline/polystyrene (PANI/PS) nanofiber-encapsulated perovskite nanocrystals for application in Schottky diodes

Harold Moremi[a], Nosipho Moloto[a], Makwena Justice Moloto[b], Arthur Moya[a]

[a]School of Chemistry, University of the Witwatersrand, Private Bag 3, Wits 2050, South Africa, E-mail: 2558157@students.wits.ac.za [b] Department of Chemistry, Durban University of Technology, P.O. Box 1334, Durban, 4000, South Africa

Keywords: PANI, Polystyrene, Schottky Diode, Nanofibers, Encapsulation

In this study, we report the synthesis and characterization of a novel hybrid nanocomposite comprising polyaniline/polystyrene (PANI/PS) nanofibers encapsulating cesium lead bromide($CsPbBr_3$) and cesium tin bromide($CsSnBr_3$) perovskite nanocrystals for application as semiconductor layers in Schottky diode devices. The perovskite nanocrystals were synthesized via a ligand-assisted reprecipitation (LARP) method, yielding highly crystalline and luminescent nanoparticles. These were subsequently embedded within electrospun PANI/PS nanofibers to form a flexible, conductive, and environmentally stable matrix. Comprehensive morphological, structural, and optical characterizations were performed using SEM, TEM, XRD, FTIR, UV-Vis spectroscopy, and photoluminescence (PL), confirming uniform encapsulation and preserved optical properties of the perovskites. Electrical characterization of fabricated Schottky diodes incorporating the composite material revealed rectifying behavior with low turn-on voltages and enhanced charge carrier mobility, attributed to the synergistic effects of the conductive PANI matrix and the perovskite's semiconducting nature. The incorporation of polystyrene provided additional thermal and environmental stability to the hybrid system [1,2]. These findings demonstrate the potential of PANI/PS-encapsulated perovskite nanocrystals as promising active layers for flexible and stable optoelectronic devices.

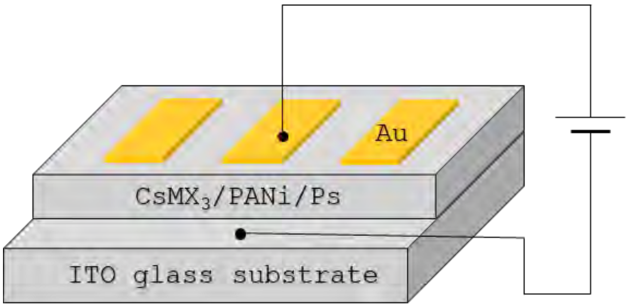


Figure 1 Schematic representation of the fabricated Schottky diode using the as-prepared PANI/PS Nanofiber-Encapsulated $CsPbBr_3$ and $CsSnBr_3$ perovkites

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Investigation of the antineoplastic activity of lantern-type diruthenium(II, III) complexes

Thato Medupe[a], *Sharon Prince*[b] *and Siyabonga Ngubane*[a]

[a]Department of Chemistry, University of Cape Town, Rondebosch, 7701, Cape Town, South Africa, E-mail: thato.medupe@uct.ac.za; [b]Department of Human Biology, Division of Cell Biology, University of Cape Town, Observatory, 7925, Cape Town, South Africa

Keywords: Breast cancer, Metallodrugs, Bimetallic ruthenium(II, III)

Breast cancer is the most prevalent malignancy and the second leading cause of death among women in South Africa, highlighting its public health impact. Conventional chemotherapeutic agents for breast cancer often cause adverse side effects, thus underscoring the need for novel therapeutic options. Ruthenium metallodrugs, which incorporate ruthenium metal centres through coordination with organic compounds or ligands, have received great attention in cancer research. This study explores the potential anti-breast cancer properties of heteroleptic diruthenium(II, III) complexes, $[Ru_2(O_2CCH_3)_3(H\text{-}ap)Cl]$ (**C1**), $[Ru_2(O_2CCH_3)_3(2\text{-}CH_3ap)Cl]$ (**C2**), $[Ru_2(O_2CCH_3)_3(4\text{-}CH_3ap)Cl]$ (**C3**), $[Ru_2(O_2CCH_3)_3(2\text{-}Fap)Cl]$ (**C4**), and $[Ru_2(O_2CCH_3)_3(4\text{-}Fap)Cl]$ (**C5**) against oetsrogen receptor positive MCF-7 and triple negative MDA-MB-231 human breast cancer subtypes, with cytotoxicity benchmarked against the commercialised drug, cisplatin.

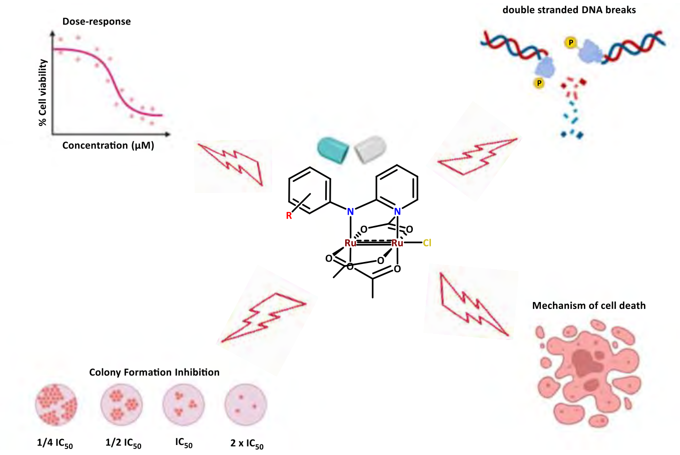

Figure: A representative image showing the investigation of cytotoxicity properties of the lantern-type diruthenium(II, III) complexes as potential anti-breast cancer agents. The representative image was created using BioRender.

C3 demonstrated promising short-term cytotoxicity and significant inhibition of MCF-7 cancer cells after 72 hours. Results obtained from colony formation assays indicate that **C3** inhibited the growth and regeneration of MCF-7 cells after 14 days of monitoring, exhibiting favourable selectivity towards MCF-7 breast cancer cells over non-malignant mammary MCF-12A epithelial cells long term. Western blot analysis suggests that **C3** induces double-stranded DNA breaks, as evidenced by increasing levels of γ-H2AX. Additionally, **C3** activated the intrinsic apoptotic cell death pathway, as demonstrated by dose-dependent increases in protein levels of cleaved caspase-9 and its downstream substrate, PARP. Altogether, these findings suggest that lantern-type diruthenium(II, III) complexes exhibit potential anti-breast cancer activity and selectivity towards oestrogen receptor positive human breast MCF-7 cancer cells and induces intrinsic apoptotic cell death pathway.

Sustainable Building Bricks From Carbon-reinforced Waste Plastic Materials

Manoko Maubane-Nkadimene[a,b], *Boitumelo Makgabutlane*[a,c], *Sabelo Mhlanga*[c], *Neil Coville*[a]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, WITS, 2050, Johannesburg, South Africa. Email: manoko.maubane@wits.ac.za. [b]Microscopy and Microanalysis Unit, University of the Witwatersrand, Private Bag 3, WITS, 2050 Johannesburg, South Africa, South Africa. [c]SabiNano Research and Innovation Division, 200 Malibongwe Drive, Randburg, 2194, South Africa.

Keywords: Carbon nanotubes, bricks, waste, plastic, fly ash

Globally, about 350 million tons of plastic waste is generated annually, with low density polyethylene, from retail industries accounting for about 49 million tons and only about 10% of the waste is recycled [1,2]. This leads to accumulation of plastic in the environment, posing a significant threat to the ecosystem. As such, there is a need to repurpose the plastic waste, and develop new useful materials, while rescuing the environment.

This study demonstrates how waste plastics and coal fly ash, which is a waste by-product from coal combustion were used to make sustainable building bricks. The bricks were reinforced with carbon nanotubes (CNTs) which are known to possess high mechanical strength that was imparted on the bricks. The CNTs were functionalized through acid treatment to improve their dispersibility in the bricks. The mechanical strength of the bricks increased with an increase in the CNT loading. All the bricks had compressive and split tensile strengths that exceeded the acceptable standards of 4 MPa and 1.2 MPa, respectively.

The reinforcement mechanism by CNTs was found to be the bridging effect and micro-void filling which allowed crack deflection rather than microcrack propagation when load was applied. The microstructure of the bricks was improved and densified, which reduced the porosity and consequently the water absorption and deformation. This offers a cheap, sustainable way to produce high quality materials, thus putting value to waste, while combating pollution for a sustainable environment and health.

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Synthesis of Pt/CdSe, Ni/CdSe, Co/CdSe, and NiCo/CdSe Janus nanoparticles for photo-electrocatalytic hydrogen generation

Tsholofelo Lepedi[a] *and Nosipho Moloto*[a]

[a]Department of Chemistry, University of the Witwatersrand, 1 Jan Smuts Avenue, 2000, South Africa, E-mail: tshololepedi@gmail.com

Keywords: hydrogen generation, Janus nanoparticles, photocatalysis, electrocatalysis

The goal of building a sustainable energy economy requires the development of clean and productive alternatives to fossil fuels. As of today, hydrogen is regarded as the leading candidate due to its high energy density and zero-carbon emission during combustion [1], [2]. Among the various hydrogen production methods such as thermochemical, electrochemical, biological, and photo-catalytic processes, photo-electrocatalytic water splitting stands out due to its potential to harness solar energy for the hydrogen evolution reaction (HER) [2]. While photo-electrocatalytic water splitting holds great promise for clean hydrogen production, its widespread adoption is dependent on the development of high performing, long lasting, and cost-effective catalysts that can drive the HER with low overpotential and high faradaic efficiency [3]. Although the semiconductor CdSe (Cadmium selenite) nanoparticles offer promising solutions for hydrogen production via photo-electrocatalysis, such as their tunable bandgap (~ 1.7 eV) and strong visible-light absorption, these characteristics are hindered by drawbacks like rapid electron-hole recombination and insufficient active catalytic sites, which restrict the overall efficiency of CdSe nanoparticles [4]. To address these challenges, semiconductor nanoparticles of cadmium selenite will be coupled with monometallic or bimetallic materials to facilitate charge separation and surface redox reactions.

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Manosylated-PVA stabilized citrus derived extracellular vesicles: A novel nano-system against non-alcoholic fatty liver inflammatory disease

Nnamdi Ikemefuna Okafor, *Yahya E. Choonara*

Wits Advanced Drug Delivery Platform (WADDP), Faculty of Health Science, School of Therapeutic Sciences, Department of Pharmacy and Pharmacology, University of the Witwatersrand, 7 York Road, 2193, Parktown, Johannesburg, South Africa.
E-mail: nnamdi.okafor@wits.ac.za

Keywords: Hesperetin, Extracellular Vesicles; Liver Inflammation; Nanosystem; Targeted Drug Delivery

Non-alcoholic fatty liver disease (NAFLD) represents a global health challenge and has a strong pathological link to obesity, prediabetes, diabetes, cirrhosis and hepatocellular carcinoma [1]. A subtype of hepatic steatosis, the first stage of NAFLD is characterized by fat deposition in hepatocytes. Most people (50–90%) who are at risk for NAFLD may develop reversible hepatic steatosis, although only a few percent (20–30%) may progress to more severe steatohepatitis and fibrosis [2]. Multiple herbal remedies, nutritional strategies, and lifestyle choices are strongly recommended for the treatment of obesity and non-alcoholic fatty liver disease [3]. Hesperetin (HST) is a naturally occurring flavonoid compound and a derivative hesperidin commonly found in citrus fruits like oranges, grapefruits, and lemons [4]. It is highly recommended due to its health-promoting effects, including its anti-inflammatory and antioxidant properties [5]. However, the use of HST is restricted due to its low stability, poor solubility and limited bioavailability [5] The development of nanocarriers and its drug encapsulation offers opportunities to overcome the limitations of HST. Notably, studies have highlighted the significant potential of HST in the intervention of ulcerative colitis [6]. However, little or no studies has explored the extraction of extracellular vesicles (EVs) for targeted delivery of HST against NAFLD. Therefore, this work is aimed at extracting EVs from oranges using ultracentrifugation, stabilized it with polyvinyl alcohol (PVA-EVs) given the hygroscopic nature of the EVs and poor stability of HST and conjugated with D-manose (Manosylated-EVs) for enhanced HST solubility and targeted delivery to the liver against NAFLD. The prepared nanosystem namely, EVs; PVA-EVs and Manosylated-EVs were characterized using various evaluation techniques. The extracted EVs demonstrated spherical morphology confirming the presence of EVs nanocarrier. The maximum solubility of PVA-EVs (923.10 µg/mL) and Manosylated-EVs (1012.27 µg/mL) in pH 5.5 and 7.4 respectively. Empty EVs, PVA-Exo and Manosylated-EVs particle sizes were 90.43, 102.34 and 123.32 nm, zeta potential: -36.12, 28.42 and -24.34 mV indicating their potential in penetrating the cells and their strong stability while showing a dispersed nanosystem with polydispersity index of 0.234 and 0.264 respectively. PVA-EVs and Manosylated-EVs exhibited entrapment efficiency 78.23 and 82.46% while releasing 78.97% and 82.8% over 24 h, respectively. The nanosystem all demonstrated an amorphous formulation signalling enhanced solubility and allows for faster dissolution and diffusion, increasing the rate at which the drug becomes available for cellular uptake and internalization These results are promising especially for enhanced bioavailability and targeted delivery of HST to the liver against NAFLD, potentially offering a more effective therapeutic strategy. However, further studies and assays are ongoing to establish the anti-inflammatory efficacy and toxicity of the nanosystem using human liver cell lines.

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Occurrence and removal efficiency of selected antibiotics in a conventional and decentralised wastewater system, Durban, South Africa

Ntombenhle Ngubane[a], *Samuel Getahun*[b], *Hogantharanni Govender*[a], *Olatunde Olatunji*[a], *and Bhekumuzi Gumbi*[a]

[a]School of Chemistry and Physics, University of Kwa-Zulu Natal, Westville,Durban, 4000, South Africa, E-mail: 220013413@stu.ukzn.ac.za [b] WASH R&D Centre, School of Engineering, University of KwaZulu-Natal, Durban, South Africa

Keywords: Wastewater treatment plant, removal efficiency, antibiotics

Antibiotics are emerging contaminants that persist in aquatic environments, posing risks to human health and ecosystems [1]. Conventional wastewater treatment plants (WWTPs) are not designed to fully remove these compounds, leading to their continuous release into surface waters. Decentralised wastewater treatment systems (DEWATS), which serve small communities, have rarely been evaluated for antibiotic removal [2,3]. This study aimed to develop and validate a sensitive analytical method using liquid chromatography–mass spectrometry coupled with solid-phase extraction for analysing sulfamethoxazole (SMX), nalidixic acid (NAL), tylosin (TYL), and norfloxacin (NOR) in wastewater. Samples were collected weekly over five weeks from a conventional Durban wastewater treatment plant (WWTP) and a decentralised wastewater treatment system (DEWATS). The method showed good performance with linear regression values of 0.99 ($R^2 > 0.99$) for all analytes, limits of detection between 0.008–0.020 mg/L, and limits of quantification between 0.025–0.060 mg/L. Recoveries (accuracy) were above 60%, and precision was below 10%, indicating good sensitivity and reproducibility. In DEWATS, SMX and NAL were detected at concentrations of 0.030–0.546 mg/L and 0.001–0.273 mg/L, respectively, while TYL and NOR were not detected. In the WWTP, TYL, NOR, and SMX were detected at concentrations of 0.078–2.492 mg/L, 0.043–0.181 mg/L, and 0.093–0.620 mg/L, respectively. These findings highlight the occurrence of antibiotics in both treatment systems and demonstrate the need for improved removal strategies to prevent environmental contamination.

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Molecular hybridisation and computational study of triazine-salicylate-anilide derivatives as potential anticancer agents and UV absorbers

Ndivhuwo R Tshiluka[a], *Kabelo P. Mokgopa*[b] *and Adeyinka S Adedapo*[a]

[a]Research Centre for Synthesis and Catalysis, Department of Chemical Sciences, University of Johannesburg, Faculty of Science, Auckland Park 2006, P.O. Box 524, Corner Kingsway Road, Johannesburg, Gauteng, South Africa, E-mail: rtshiluka@uj.ac.za [b]*Department of Chemistry, Rhodes University, Makhanda/Grahamstown 6140, South Africa*

Keywords: Triazine-Salicylate-Anilide, Computational methods, Anticancer agents, UV absorbers

Cancer is the second leading cause of death worldwide, accounting for nearly 10 million deaths in 2020, or nearly one in six deaths.[1] On the other hand, the effects of the ozone layer have increased the amount of radiation that reaches the Earth's surface, which is highly harmful to human health, according to reports.[2] Considering the impacts and threats of Cancer and UV radiation to human life, there is still an urgent need for the development of new cancer drugs and UV absorbers.[3] Hence, in our present study, we have used molecular hybridisation to design a new series of hybrid Triazine-salicylate-anilide **4** derivatives as shown in **Figure 1**. The synthesized hybrids **4** were characterised by NMR, FTIR and HMRS spectroscopies, whereas a computational approach was carried out using molecular docking, dynamics, MMGBSA, ADMET and DFT studies. The anticancer screening of our target compounds will be done in collaboration with CSIR, whereas the UV absorption study of these compounds will be carried out using a UV spectrophotometer in collaboration with Mintek.

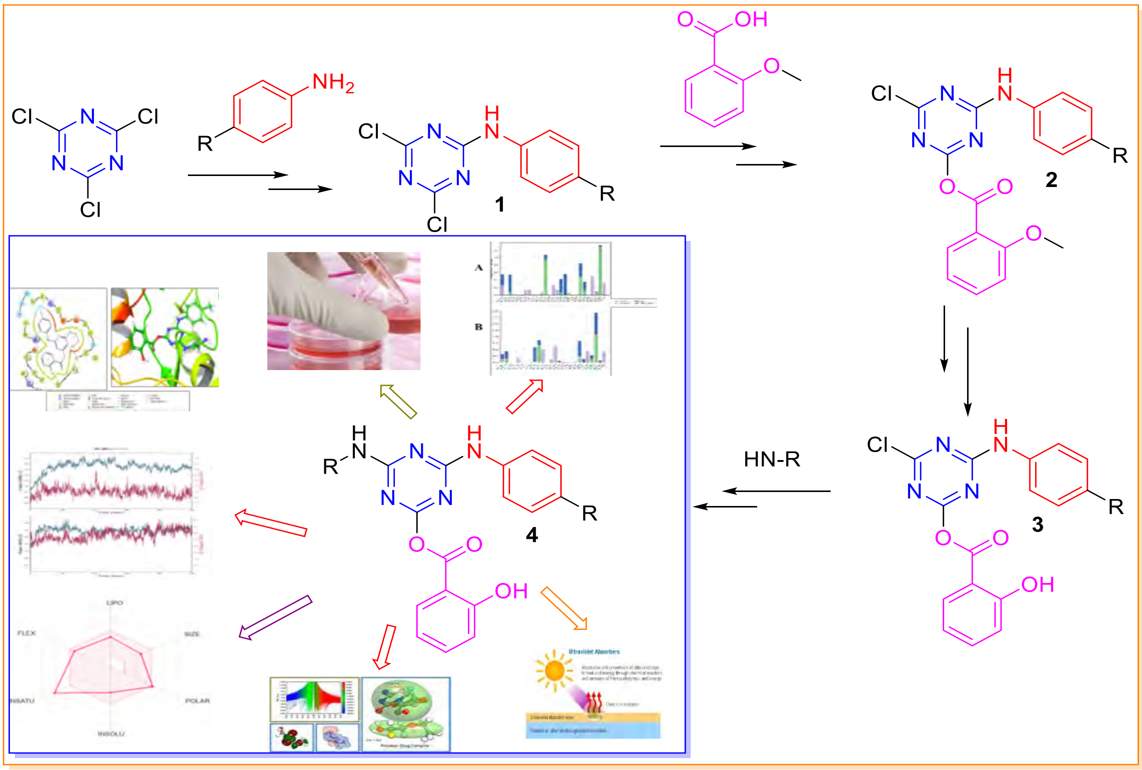

Figure 1: Synthesis of triazine-benzotriazole-salicylate hybrids

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Phytochemical screening using UHPLC–Q/Orbitrap/MS to study antioxidant and toxicity potential of *Lippia multiflora* Moldenke

Bafedile Tlhapi[a], *Ntsoaki Malebo*[a], *Idah Manduna*[a], *Monizi Mawunu*[b] *and Christinah Chokwe*[c]

[a]Centre for Applied Food Sustainability and Biotechnology, Faculty of Health and Environmental Sciences, Central University of Technology, Bloemfontein 9300, South Africa, E-mail: btlhapi@cut.ac.za; nmalebo@cut.ac.za; imanduna@cut.ac.za. [b]Department of Agronomy, Polytechnic Institute, Kimpa Vita University, Luanda P.O. Box 77, Angola E-mail: m.mawunu2000@gmail.com [c]Department of Chemistry, College of Science Engineering and Technology, University of South Africa, Florida, Johannesburg, 1710, South Africa E-mail: chokwrc@unisa.ac.za

Keywords: *Lippia multiflora*; chemical profile; phytochemical compositions; antioxidant activity; cytotoxicity; total flavonoid content, total phenolic content

Lippia multiflora Moldenke is a member of the Verbenaceae family. Aerial and underground parts of *Lippia multiflora* are commonly used by traditional healers in Angola and other African countries for the treatment of many infectious diseases. [1-2] Ethnopharmacological studies have indicated antioxidant activities; as well as the cytotoxicity of the crude extracts.[3] However, there are few studies which have linked the phytochemistry to the pharmacological activities. This study aimed at exploring the phytochemistry and pharmacological properties of *L. multiflora*. It focuses on the crude leaf, root and stem bark extracts, using UHPLC–Q/Orbitrap/MS, and shows antioxidant and toxicity assessments.

Methodology: Chemical characterization of the leaf, stem bark and root of *L. multiflora* was assessed through quantification of total phenolic and flavonoid contents followed by Q exactive plus orbitrap™ ultra-high-performance liquid chromatography-mass spectrometer (UHPLC-MS) screening. The correlation between the extracts and the correlation between the compounds was studied using the multivariate analysis. Furthermore, the antioxidant activities of the crude extracts were carried out "*in vitro*" using DPPH (2,2-diphenyl-1-picrylhydrazyl) free radical scavenging and reducing power assays; while the *in vitro* toxicology was evaluated using the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay.

Results: A total of 20 compounds were tentatively identified from different plant parts of *L. multiflora* using UHPLC–Q/Orbitrap/MS. In the antioxidant activity, the leaf extract (IC_{50} = 0.559 ± 0.269 µg/mL) and stem bark extract ($IC_{0.5}$ = 0.029 ± 0.026 µg/mL) had the highest DPPH free radical scavenging activity and reducing power capacity. High phenolic and flavonoid content was found in the leaf extract (32.100 ± 1.780 mg GAE/g) and stem bark extract (624.153 ± 29.442 mg QE/g), respectively. The results further showed that the stem bark, and leaf extracts were well-tolerated by the Vero cell line at concentrations up to 50 µg/mL. Multivariate analysis of the data obtained indicated that the chemistry of the stem bark and root are similar and different from the chemistry of the leaf.

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Isocyanide-based Ugi-multi-component (U-MCR) synthesis of 3-indole-tetrazoles and their anti-HIV evaluation

Mashaole T.C Ragedi[a*], *Darian Naidu*[b], *Oluwatoba Oyeneyin*[a], *Nompumelelo Mkhwanazi*[b], *Matshawandile Tukulula*[a]

[a] School of Chemistry and Physics, College of Agriculture and Engineering, University of KwaZulu Natal, Westville, Private Bag X54001, Durban, 4000, South Africa.

Keywords: 3-Indole-tetrazoles, U-MCR, HIV-1 subtype B, Time of addition studies, molecular docking.

Over 36 million individuals are living with HIV, and over 39 million fatalities are attributable to HIV/AIDS to date. HIV/AIDS continues to have a catastrophic impact on people's health throughout the world [1]. When the HIV undergoes mutations that render it less susceptible to the effects of antiretroviral drugs, it leads to the emergence of drug resistance in HIV treatment [2]. Thus, there is an urgent need to find new treatment regimens that will be effective against both resistant and non-resistant strains. To this end, a series of new 3-Indole tetrazole derivatives (Figure 1) were synthesised in a single pot *via* the isocyanide-based Ugi multicomponent reaction in 35 to 73 % yields. The synthesised compounds were fully characterised using 1D and 2D NMR, IR, and their purity was checked by HPLC. Their antiviral activities were evaluated *in vitro* against HIV-1 subtype B virus on Luciferase-based antiviral assay on TZM-bl cell-lines, with azidothymidine (AZT) used as a reference drug. The time of addition revealed these compounds to be potent attachment inhibitors with moderate activity against the reverse-transcriptase enzyme. The majority of the compounds displayed acceptable cytotoxicity profile while molecular docking studies revealed interesting interactions with amino acid residues with HIV surface glycoprotein 120 and reverse-transcriptase enzyme active sites.

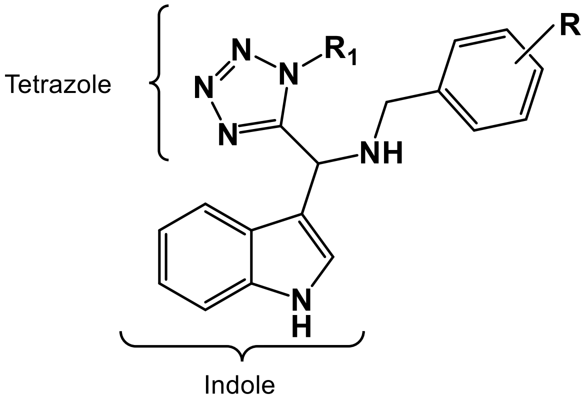

Figure 1: 3-Indole-tetrazole target compounds

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Novel pyrazoline-benzoxaborole hybrids: Design, synthesis and in silico analysis

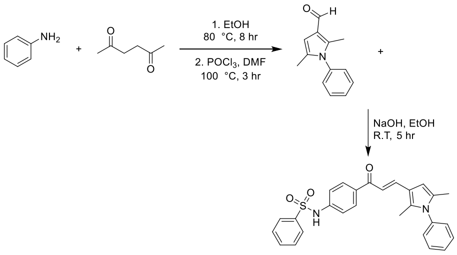
Nosipho Biyela[a], *Mokhitli Morake*[b], *Setshaba Khanye*[a]

[a]Division of Pharmaceutical Chemistry, Rhodes University, Makhanda, 6139, South Africa, Email:g19b1387@campus.ru.ac.za. School of Life Sciences, University of Dundee, Dundee, Scotland

Keywords: Benzoxaborole, pyrazolines, malaria, molecular hybridization, computer-aided drug design

Malaria remains a significant health concern, particularly in Africa, where *Plasmodium falciparum* (*P. falciparum*) is the most virulent causative agent of the disease. The upsurge of antimalarial drug resistance hinders malaria treatment, highlighting the urgent need for innovative therapeutics [1]. Pyrroles are a privileged scaffold in medicinal chemistry due to their widespread presence in biologically active compounds and their structural adaptability, allowing for diverse chemical modifications [2]. Another versatile scaffold is Sulfonamide, since its adaptability allows for modifications. Furthermore, it has essential biological activities and distinctive physicochemical properties [3]. Herein, we propose using structure-based drug design and molecular hybridization, a widely used technique in medicinal chemistry, to identify pyrrole-sulfonamide hybrids with potent antiplasmodial activity as potential inhibitors of falcipains, the essential cysteine proteases produced by the malaria parasite.

Pyrazoline-benzoxaborole hybrids were designed using quantitative structure-activity relationship analysis. **Scheme 1** depicts the synthetic route to access the target compounds.



Scheme 1: Synthetic approach to accesss pyrrole-sulfonamide hybrids.

The key intermediates and a subset of the target compounds have been successfully synthesized and characterized, using 1H and 13C NMR and FT-IR spectroscopy. *In silico* docking studies demonstrated that the target compounds exhibit strong binding affinity, supporting their potential as falcipian binding inhibitors and as potential antiplasmodial agents.

The predicted physicochemical and pharmacokinetic properties suggest that the compounds possess drug-like properties. The target compounds will be screened against drug-sensitive and drug-resistant strains of *P. falciparum*, and compounds exhibiting promising activity will be assessed for cytotoxicity.

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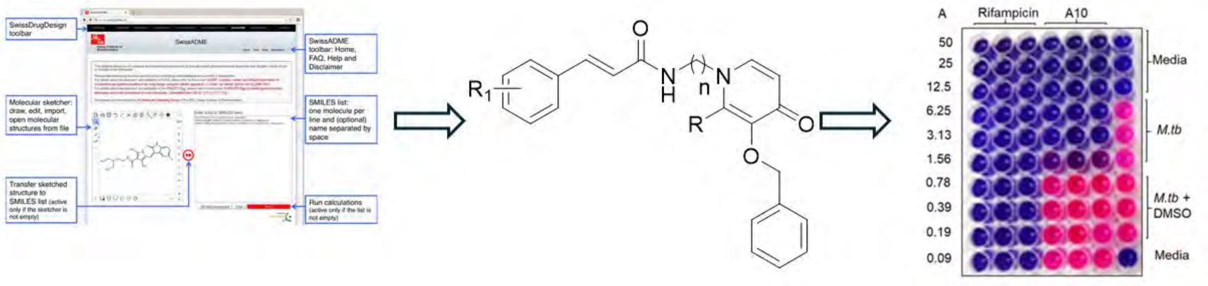
Design and synthesis of novel hydroxypyridinone-cinnamic acid hybrids

T. Malusela[a], S.S. Mnyakeni-Moleele[a], N. Gama[b] and M.V. Bvumbi[a]

[a]Department of Chemistry, University of Venda, University Rd, Thohoyandou, 0950, South Africa, E-mail: thisundiwimalusela@gmail.com.
[b]Department of Biochemistry, Genetics, and Microbiology, University of Pretoria, Lynnwood Rd, Hatfield, Pretoria, 0002 South Africa

Keywords: Synthesis, Hydroxypyridinones, Cinnamic acids, Hybrids

The global burden of tuberculosis (TB), exacerbated by the emergence of multidrug-resistant (MDR) and extensively drug-resistant (XDR) Mycobacterium tuberculosis (Mtb) strains, underscores the urgent need for new chemotherapeutic agents with novel mechanisms of action.[1] In this study, we report the design, synthesis, and biological evaluation of a new class of hybrid molecules combining hydroxypyridinone and cinnamoyl scaffolds, two pharmacophores known for their metal-chelating and antimicrobial properties. The design and synthesis of these compounds were achieved by a molecular hybridization strategy, which involves the combination of pharmacophoric moieties of bioactive substances to produce a new hybrid compound with improved affinity and efficiency.[2] A small hydroxypyridinone–cinnamoyl hybrids library was synthesized using modular coupling strategies, allowing for structural variation on both moieties. The synthesized compounds were characterized by spectroscopic methods (NMR, IR, and MS). The compounds were then screened against *M. tuberculosis* H37Rv using a microdilution assay to determine their minimum inhibitory concentrations (MICs). The screening results showed no significant antimycobacterial activity, with MIC values exceeding 60 µM. Although the hybrids did not exhibit potency at the tested concentrations, the findings highlight structural limitations and offer insights for future scaffold refinement. This study contributes to understanding structure–activity relationships in hydroxypyridinone and cinnamoyl-based compounds for TB drug discovery.



In silico analysis Synthesized compound Biological evaluation

Figure 1: Designed proposed compounds in silico (SWISSADME software) and biological evaluation of compounds against *M. tuberculosis* H37Rv using a microdilution assay to determine their minimum inhibitory concentrations (MICs).

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Design and synthesis norbornane-based derivatives targeting amyloid-β, AChE, and oxidative stress as a potential Alzheimer's disease treatment

Ramba[a] *Egunlusi*[b]*and Khanye*[a]

Faculty of pharmacy, Rhodes University, Makhanda, 6139, South Africa, E-mail: Ayodeji.egunlusi@ru.ac.za

Keywords: norbornane, anticholinesterase, Alzheimer's disease, amide formation, multi-target ligand

Alzheimer's disease (AD) is a progressive neurodegenerative disorder characterized by memory loss, cognitive decline, and behavioral changes, affecting over 50 million people globally [1]. Despite significant research efforts, effective treatments to halt or reverse progression of AD remain elusive. [2]. This may be attributed to the single-target approach used for AD, a complex and multifactorial disease. Therefore, a multi-target approach could prove more beneficial [3]. This project focuses on the design and synthesis of norbornane-based derivatives targeting amyloid beta aggregation, acetylcholinesterase inhibition, and oxidative stress pathways, with the aim of developing potential multifunctional therapeutic agents for Alzheimer's disease.

Cycloaddition reaction between maleic anhydride and monomerised cyclopentadiene afforded a norbornane scaffold (carbic anhydride). Under reflux conditions, a linker (ethylenediamine) was incorporated into the norbornane scaffold to form an intermediate. In the presence of sulfuric (H_2SO_4), as a catalyst, the intermediate underwent an amidation reaction with a series of carboxylic acid derivatives, producing the final products in favourable yields. The final products were characterised by proton NMR and FT-IR.

FT-IR analysis confirmed amide bond formation, evidence by characteristic N-H stretching vibrations (3110-3500 cm^{-1}) and C=O stretches (1650-1680 cm^{-1}). In the proton NMR spectra, the characteristic bridge protons of the norbornane scaffold appeared as a doublet of triplets and doublet between 1.5 -2 ppm across all compounds. The CH_2 peaks observed between 2.5-3.0 ppm confirmed the formation of the intermediate, while the presence of aromatic proton signals (δ 7-8 ppm) indicated successful incorporation of the carboxylic acid derivatives.

FT-IR confirmed amide bond formation with characteristic N-H (3110-3500 cm^{-1}) and C=O (1650-1680 cm^{-1}) stretches. The CH_2 (δ 2.5-3.0 ppm) confirms as the present of the linker. The presence of aromatic ring peaks (δ 7-8 ppm) that suggest acid were successfully incorporated.

Of the 30 proposed compounds, 4 have been successfully synthesized. Upon completion of the full series, further biological evaluations will include Thioflavin T (ThT) fluorescence assays (to assess anti-Aβ aggregation activity), antioxidant and anticholinesterase assays, as well as cytotoxicity screening. In addition, in silico studies, including molecular docking and SwissADMET will be conducted to support the biological findings, elucidate potential molecular mechanisms, and predict drug-likeness and pharmacokinetic properties. Upon completing this study, we hope to have successfully developed multifunctional agents or lead compounds for the treatment of Alzheimer's disease. This could significantly impact global health by providing new avenues for AD treatment, ultimately improving patient outcomes and alleviating the socio-economic burden associated with this devasting disease.

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Molecular hybridisation and *in silico* studies of triazine-anilide derivatives as potential anticancer agents

Phumzile. N. Mqilingwa[a], *Sithandile Ngxangxa*[b] *and Ndivhuwo. R. Tshiluka*[c]

Research Centre for Synthesis and Catalysis, Department of Chemical Sciences, University of Johannesburg, Faculty of Science, Auckland Park 2006, P.O Box 524, Corner Kingsway Road, Johannesburg, Gauteng, South Africa nomvulamqilingwa2310@gmail.com

Keywords: molecular hybridisation, triazine-anilide derivatives, anticancer agents

Cancer is one of the leading causes of death globally, with the World Health Organization (WHO) estimating that in 2020, there were nearly 10 million cancer-related deaths [1], and an estimated 19.3 million new cases in the same year [2]. Current existing treatments such as radiotherapy and surgery often have severe side effects such as damage to DNA caused by ionising radiation and potential complications such as infections and challenges in post-surgical recovery [3]. These challenges highlight the need for novel therapeutic methods which are more selective and effective. Molecular hybridisation is a concept based on the combination of pharmacophores from different bioactive molecules, resulting in novel hybrid compounds with improved efficacy and efficiency compared to their parent compounds [4]. This study uses molecular hybridisation as an approach to synthesise triazine-anilide hybrids **5**, as shown in figure **1**, and to explore their potential as anticancer agents. These compounds were characterised using techniques such as NMR, FTIR, and HRMS. *In Silico* studies such as ADMET, density functional theory (DFT) and molecular docking, were conducted to predict the binding affinities and stabilities of these triazine-anilide hybrids and to understand their charge-charge interactions and their inhibitory potential [5] against breast cancer cell lines. This research aims to pave the way for the development of new therapeutic strategies that enhance efficacy and minimise side effects and contribute to the existing body of knowledge to inform future research in the search for a cancer cure.

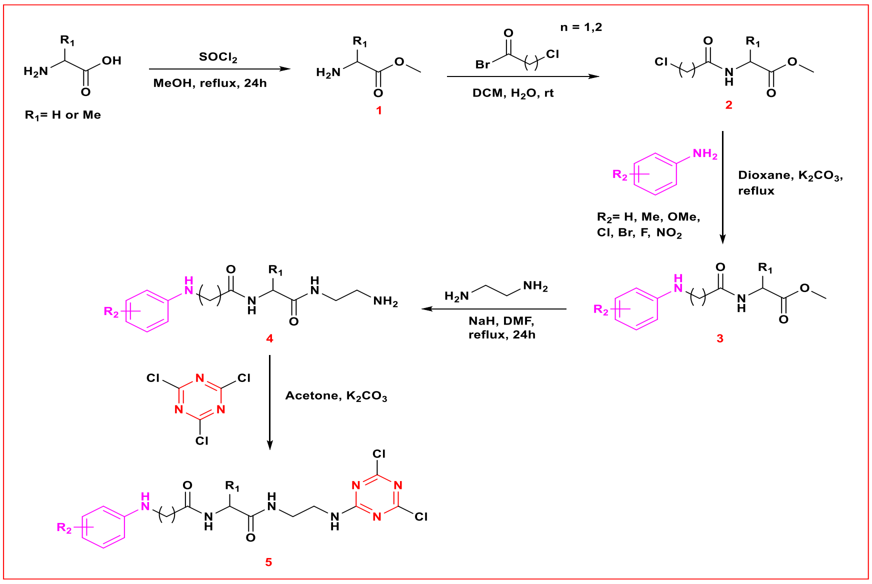

Figure 1: Synthesis of triazine-anilide hybrids

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Continuous flow synthesis of indenone derivatives

Simamkele Mayoli, Paul Watts, Faith Akwi

Department of Chemistry, Nelson Mandela University, PO Box 77000, Port Elizabeth, 6031, South Africa
E-mail: s223318493@mandela.ac.za

Keywords: indenone, flow chemistry, medical, synthesis

Substituted indenones have vital biological properties and play a significant role in medical drug synthesis. These biological properties include anticancer, antioxidant, antimicrobial, anti-inflammatory[1] and AlkBH3 inhibitory activity. There has been an increase in demand for procedures that are safer and greener, the pharmaceutical industry has been focusing on possible technologies to reach shorter reaction time and quicker scale-up procedures[2].

Under controlled conditions, flow chemistry approach has made it possible to synthesize these compounds in higher yields, safely[3] and quicker compared to batch methods. In batch chemistry, synthesis of indenone derivatives takes days while the products can be synthesized within an hour in continuous flow chemistry. Continuous flow chemistry made it possible to synthesize the indenone derivatives by using telescoping methods[4],[5]. Two-step reactions were carried out continuously without quenching and purifying in-between steps whereas these were done in batch synthesis. ln this study, indenone derivatives, 1H-inden-1-one, 4-methyl-1H-inden-1-one, 2-bromo-1H-inden-1-one, 3-bromo-1H-inden-1-one, 3-chloro-1H-inden-1-one and 2-chloro-1H-inden-1-one are synthesized in continuous flow chemistry. These indenone derivatives that are used as intermediates in the synthesis of medical drugs.

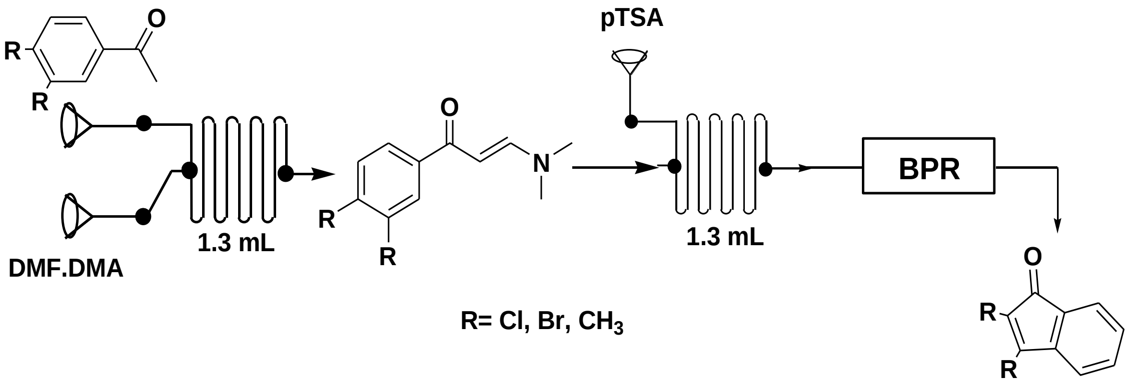

Figure 1: Continuous flow reaction set-up.

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Encapsulation and controlled release of halogenated natural products in nanoformulations for enhanced stability and biological activity

Ritshidze Mudanabula[a], *Edith Antunes*[b] *and Denzil Beukes*[a]

[a] School of Pharmacy, University of the Western Cape, Bellville, 7535, South Africa, E-mail: 4494770@myuwc.ac.za.
[b]Department of Chemistry, University of the Western Cape, Bellville, 7535, South Africa

Keywords: Halogenated natural products, Solid lipid nanoparticles, Nanoencapsulation, Antimicrobial activity

Halogenated natural products are bioactive compounds derived from natural sources (e.g., marine organisms, plants, fungi) that contain halogen atoms. These halogen groups often enhance biological activity, stability, and membrane permeability. Marine-derived halogenated natural products, particularly those from *Plocamium ssp*. are recognized for their potent biological activities, including notable antimicrobial effects. However, the therapeutic development of these compounds is often hindered by challenges related to their lipophilicity, poor solubility and limited stability under physiological conditions. This study aimed to address these limitations through the development of lipid-based nanoparticle formulations to enhance the solubility, stability, and biological efficacy of polyhalogenated compounds.

Halogenated natural products were extracted and characterized from *Plocamium spp*. using established chromatographic and spectroscopic techniques. These bioactives were encapsulated into solid lipid nanoparticles (SLNs) using the hot homogenization method. The physicochemical properties of the resulting SLNs were characterized by dynamic light scattering (DLS) to determine particle size, polydispersity index (PDI), and the zeta potential parameters. The surface morphology were examined using scanning and transmission electron microscopy (SEM and TEM), while the entrapment efficiency was assessed via nuclear magnetic resonance (NMR) spectroscopy.

In addition, the antimicrobial activity was assessed using the broth micro dilution and disc diffusion methods to evaluate the efficacy of the encapsulated halogenated natural products against selected microbial strains, *Escherichia coli* (*E. coli*) and *Staphylococcus aureus* (*S. aureus*). These tests determined the minimum inhibitory concentration (MIC) and the zone of inhibition, which provided insight into the antimicrobial potential of the nanoformulated compounds. This approach was expected to improve stability and therapeutic potential of halogenated natural products to enable their use in clinical and pharmaceutical applications. These findings will contribute to the development of effective drug delivery systems for marine-derived bioactive compounds and also support their use in antimicrobial drug development.

Thermo-responsive chitosan–agarose nanohydrogel for nano-enabled personal care product formulation

Mandisa Mathenjwa[a], *Florence Lehutso*[b], *Yolanda Tancu*[b] *and Bhekumuzi Gumbi*[a]

[a]Department of Chemistry and Physics, University of KwaZulu-Natal, Westville Campus, Durban, 4000, South Africa, E-mail: 219004850@stu.ukzn.ac.za. [b]Council for Scientific and Industrial Research, Water Research Centre, Meiring Naudé Road, Brummeria, Pretoria, 0001, South Africa

Keywords: Silver nanomaterial, Chitosan-Agarose Nano-Silver hydrogel, Nano-enabled Personal Care Product, thermo-responsive technology

Silver nanoparticles (nAg) in nano-enabled products (NEPs) are mostly used in consumer products because of their broad range of antibacterial capabilities against pathogenic microorganisms [1]. Because of this, these NPs have been successful as preservatives in the personal care, health and fitness industries' shampoos, kinds of toothpaste, anti-acne cosmetic formulas, and other similar items [2,3,4,5]. The nAg are not permanently fixed to the NEPs matrix and have been shown to have varying degrees of environmental exposure potential, ranging from minimal to high, reliant on various factors [6]. Thus, release exposure potentials of nAg from NEPs should be considered at the formulation stages. Herein, the current study aimed to produce a thermo-responsive chitosan-agarose hydrogel, engineered with citrate-capped nAg to facilitate the dynamic release and reabsorption of silver in aqueous environments. The thermo-responsive hydrogel synthesised by co-polymerisation, which undergoes reversible sol-to-gel transitions in response to temperature changes, is designed to optimize the retention and release of nAg in water-based applications. The characterization of the chitosan–agarose hydrogel using high resolution transmission electron microscopy (HRTEM) coupled with energy-dispersive X-ray spectrometry (EDX), X-ray diffraction (XRD), Fourier transform infrared (FTIR), TGA and silver loading and entrapment tests highlights the hydrogel's ability to reabsorb nAg at room temperature (25 °C) from aqueous solutions and release them in a controlled manner upon temperature shifts to 50 °C. This behaviour is crucial for applications in personal care products, where precise control over silver delivery is desired. This innovative approach leverages thermo-responsive technology to enhance the functionality and sustainability of silver-enriched personal care products.

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Synthesis of the resurrection plant metabolite 3,4,5-tri-*o*-galloylquinic acid

Sinoxolo Madasi[a], *Marwaan Rylands*[a], *Roger Hunter*[a] *and Nonhlanhla Khumalo*[b]

[a]Department of Chemistry, University of Cape Town, Rondebosch, Cape Town, 7701, South Africa. [b]Department of Medicine, University of Cape Town, Observatory, Cape Town, 7925, South Africa. Email: mdssin002@myuct.ac.za.

Keywords: *Myrothamnus flabellifolius*, antioxidants, natural products, organic synthesis

The phytochemical 3,4,5-tri-*O*-galloylquinic acid (TGQA) is a plant metabolite commonly found in various plant species.[1] One such species that has been shown to have high concentrations of (TGQA) is *Myrothamnus flabellifolius*.[1] The extracts of this well-known Southern African resurrection plant display a wide range of promising medicinal properties,[2] however, because of the complex composition of the plant extracts, these properties could not be well studied or quantified.[3]

This project focused on the synthetic preparation of 3,4,5-tri-*O*-galloylquinic acid, the major antioxidant reported in *Myrothamnus flabellifolius*. The synthesis employed a carbodiimide-mediated esterification as a key step, starting from quinic and gallic acids. Quinic acid was first converted to benzyl quinate, which was then reacted with *O*-protected tri-benzyloxygallic acid to form the benzyl protected tri-ester.

The tri-ester was obtained using *N,N′*-Dicyclohexylcarbodiimide (DCC) as the coupling reagent; however, the product contained Dicyclohexylurea (DCU) as an inseparable impurity. In contrast, coupling with 1-Ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC) yielded the tri-ester in reduced yield (18%) but without the urea by-product. Global deprotection of both the benzyl ester and benzyloxy ethers afforded the product (TGQA) in an overall yield of 17%.

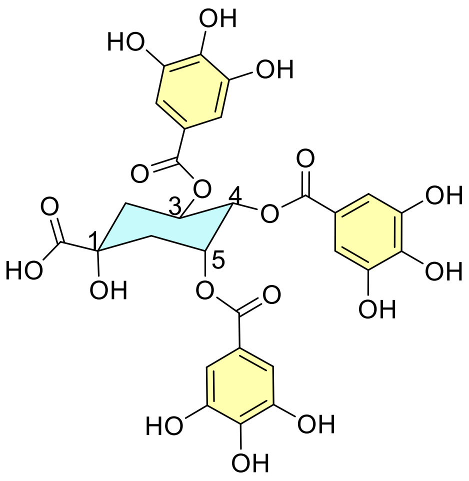

Figure 1: The target compound 3,4,5-tri-*O*-galloylquinic acid (TGQA) structure.

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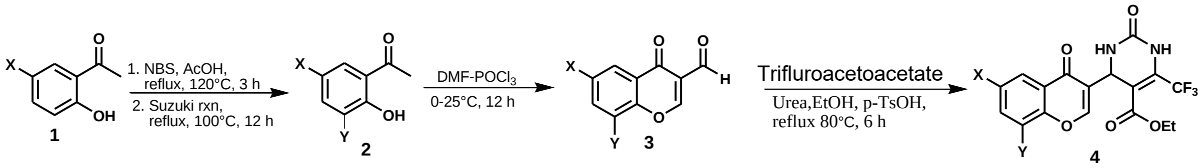
Synthesis of chromone-3-carbaldehyde derivatives as potential antituberculosis agents

Phophi H[a], *Ramaite I.D.I*[a], *Van Ree T*[a] *and Ganto M.M*[a]

[a]Department of Chemistry, University of Venda, Thohoyandou 0950, South Africa, E-mail: hlamulo.phophi@gmail.com

Keywords: Chromones, Pyrimidine, Suzuki, Tuberculosis

Tuberculosis (TB) remains a significant public health challenge worldwide. The rise in multidrug-resistant (MDR) and extensively drug-resistant (XDR) TB cases complicates treatment efforts and increases the risk of spread.[1] Despite advances in science, there is a need for effective and diverse therapeutic alternative treatments. Preliminary studies suggest that Chromone-3-carbaldehyde derivatives exhibit a wide range of biological activities, making them viable candidates as anti-tuberculosis agents.[2] The substantial structure-activity Relationships (SAR) studies of chromone skeleton show that substitutions at C-3, C-6, and C-8, and the use of electron-withdrawing groups (EWGs) can contribute to anti-tubercular activity.[3] Derivatives of 2-hydroxyacetophenone were successfully synthesized through a Suzuki coupling reaction and characterized using spectroscopic techniques and physical data. The synthesized acetophenones were then subjected to a Vilsmeier-Haack reaction, leading to the formation of chromone-3-carbaldehyde derivatives. These compounds were synthesized and purified using column chromatography, achieving yields ranging from 40-98%. The compounds were synthesized following the synthetic Scheme 1. The synthesized chromone-3-carbaldehyde derivatives are to be sent for biological screening at H3D to evaluate their biological activity and efficacy as antituberculosis agents.



Scheme 1: Reaction scheme of chromone derivatives

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An investigation of the herbicidal activity of *Coleus neochilus* Schltr

<u>Delisile F. Zulu</u>, Fanie R. van Heerden and Muvhango Rasalanavho

[a]School of Agriculture and Science, Discipline of Chemistry, University of KwaZulu-Natal, Pietermaritzburg, 3209, South Africa, E-mail: 217045966@stu.ukzn.ac.za

Keywords: Herbicides, *Coleus neochilus*, Phytotoxicity

Most synthetic herbicides used in the agricultural sector to control weeds can cause environmental pollution [1]. The identification and quantification of bioactive compounds from plant extracts with phytotoxic properties can contribute to the development of environmentally friendly herbicidal agents.

In this project, extracts of *Coleus neochilus* Schltr., belonging to the Lamiaceae family, were assayed for phytotoxicity to identify biologically active compounds that can serve as alternatives to currently used synthetic herbicides. The DCM-MeOH crude extract of the leaves of *C. neochilus* showed positive inhibition on the germination of lettuce (*Lactuca sativa*) seeds. This crude extract was further fractionated into five fractions, which were assayed for phytotoxicity, resulting in the identification of two active fractions. The EtOAc was the most active fraction, and we have identified the two major compounds as abietene diterpenoids (Figure 1) by LC-MS. The next step in our project is to isolate the compounds, confirm the structures by NMR spectroscopy, and assay the compounds for the inhibition of seed germination.

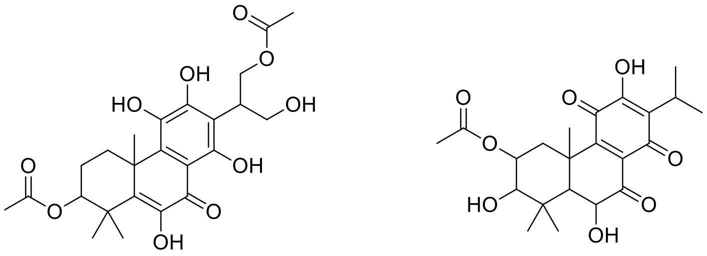

Figure 1. The abietane diterpenoids identified in *Coleus neochilus*.

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Structural and synthetic investigations of halogenated natural products from *Plocamium* species

Eldon P. Damon[a], *Edith M. Antunes*[b] *and Denzil R. Beukes*[a]

[a] School of Pharmacy and [b] Department of Chemistry, University of the Western Cape, Bellville, 7535, South Africa, E-mail: 3512610@myuwc.ac.za

Keywords: halogenated natural products, stereochemistry, NMR, ECD, marine natural products

Chiral halogenated natural products represent a structurally diverse and biologically significant class of compounds, with over 800 known examples exhibiting potent antimicrobial, cytotoxic, and neuroactive properties. Many of these compounds are derived from marine organisms, particularly red algae of the genus *Plocamium*. Despite their prevalence, determining the absolute configuration of halogen-bearing stereocentres remains a major challenge, due to the subtle influence of halogen atoms on chiroptical properties and the scarcity of reference standards.

Electronic circular dichroism (ECD) spectroscopy, when combined with density functional theory (DFT)-based spectral prediction, offers a powerful approach for the assignment of absolute configuration. ECD measures the differential absorption of left- and right-circularly polarized light by chiral molecules and is particularly suited to compounds with UV-active chromophores. In addition to stereochemical complexity, halogenated natural products are often chemically reactive, undergoing elimination and substitution reactions with biological nucleophiles, which may contribute to their mode of action.

In this study, halogenated monoterpenes were isolated from *Plocamium cornutum* and *Plocamium corallorhiza* collected from South African coastal regions. Following structure elucidation by 1D and 2D NMR, the absolute configuration of selected compounds was determined by comparison of experimental and DFT-calculated ECD spectra. Chemical reactivity was assessed through derivatization with phenylhydrazine and other nucleophiles, revealing novel transformations including the formation of pyrazole analogs.

These findings highlight the utility of ECD in resolving halogen-bearing stereocentres and demonstrate that halogenated natural products may serve as versatile scaffolds for synthetic elaboration. This dual exploration of structure and reactivity contributes to our understanding of how subtle stereoelectronic features in marine metabolites govern their biological activity and synthetic potential.

Preparation and investigation of coumarin-based chemosensors towards the sensing of ions using UV studies in aqueous systems

Tyla Kotze and Neliswa Mama

[a]Department of Chemistry, PO Box 77000, Nelson Mandela University, Gqeberha, 6031, South Africa, E-mail: s217522475@mandela.ac.za.

Keywords: Coumarin, Chemosensor, Ether, Ester, Selectivity and UV studies.

This project involves the synthesis of six different coumarin-based ether derivatives (**E2-E5**) and coumarin-based ester derivatives (**H1-H2**). FT-IR, 1H NMR and 13C NMR were used to confirm the structures of all these compounds. The abilities of these novel compounds as chemosensors for detection of cations and anions were investigated using UV-visibility analysis. These compounds displayed favorable interactions with Fe^{2+} and Fe^{3+} ions with an increase in absorbance. Ether derivatives **E2-E5** did not display any degree of selectivity or sensitivity towards the chosen anions. It was found that in the presence of FeCl$_2$, sensors **H1** and **H2** displayed a degree of selectivity and further investigations were therefore carried out. From the titration experiments, the limit of detection, limit of quantification and association constants were determined. Job's plot analyses were also constructed to determine the binding ratios, which was supported by Benesi-Hildebrand studies. The binding ratio between the sensors and metal cations during complexation was found to be 1:1. Reversibility studies were carried out using EDTA to determine whether the sensors could be reused. Molecular Modelling studies were used to determine the preferred binding sites. Lastly, real-life application screenings were also done to determine if the sensors will be able to be used in real-life scenarios.

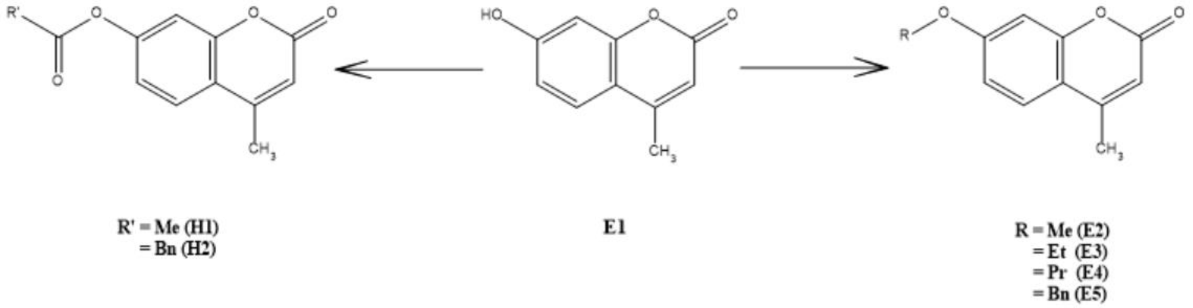

Figure 1: Structures of coumarin-ether derivatives E2-E5 and coumarin-ester derivatives H1-H2

An investigation on South African medicinal plants with herbicidal effect

Aphiwe B. Sishi, Fanie R. van Heerden and Muvhango Rasalanavho

School of Agriculture and Science, Discipline of Chemistry, University of KwaZulu-Natal, Pietermaritzburg, 3201, E-mail: 220087317@stu.ukzn.ac.za

Keywords: Herbicidal activity, Phytochemistry, Bioassays, *Hilliardiella*, *Helichrysum*

Synthetic herbicides are widely used, but overapplication has led to environmental pollution, herbicide-resistant weed biotypes, and adverse effects on non-target organisms. These challenges necessitate the exploration of safer, biodegradable alternatives. In this context, plant-derived natural products offer a sustainable and ecologically compatible solution [1]. This study investigates the herbicidal potential and isolation of herbicidal compounds from four South African medicinal plants: *Hilliardiella capensis*, *Hilliardiella aristata*, *Helichrysum pandurifolium*, and *Helichrysum nudifolium*. These species were selected due to their traditional medicinal relevance and known production of bioactive secondary metabolites. The dried roots, stems, leaves, and flowers were sequentially extracted with hexane (Hex), dichloromethane (DCM), and methanol (MeOH). The phytotoxic activity was assayed by observing the inhibition of the germination of seeds (*Lactuca sativa*) [2].

Among the extracts assayed, the DCM extracts showed the highest inhibitory activity on seed germination. Extracts demonstrating significant phytotoxicity were fractionated using SPE DIOL columns, and further bioassays were performed to identify active fractions. The viability of the seeds and controls confirmed the assay's reliability. The bioassay-guided fractionation led to the isolation and structural elucidation of active compounds. GC-MS, LC-MS, and ^{1}H NMR spectroscopy are being used to characterize the active compounds. Results support the hypothesis that these plant species contain herbicidal compounds with potential for natural herbicide development.

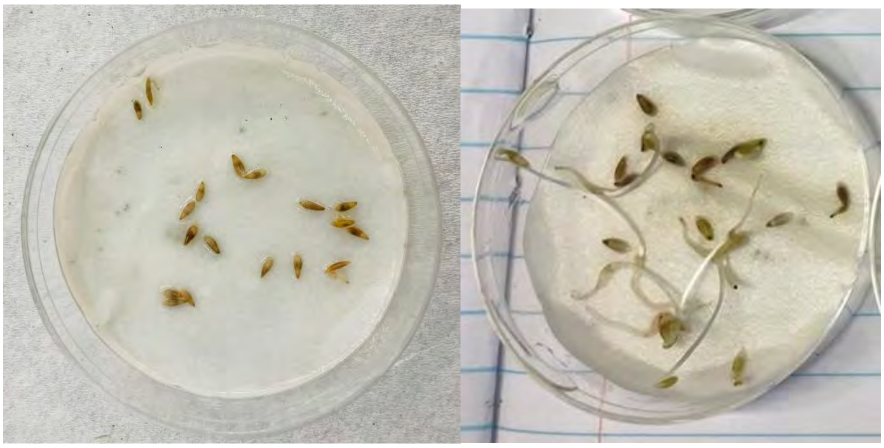

Figure 1: The phytotoxic bioassays of crude extracts.

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Design and Synthesis of Novel Quinoline-Ferrocene Hybrids as Anti-Tuberculosis Agents

Delight Chaka[a], Setshaba D. Khanye[a]

[a]Division of Pharmaceutical Chemistry, Faculty of Pharmacy, Rhodes University, PO Box 94, Makhanda, Eastern Cape, 6140, South Africa, E-mail: g20c1316@ru.ac.za.

Keywords: tuberculosis, quinolines, benzoxaboroles, *Mtb*-LeuRS and *Mtb*ATPase enzymes

Tuberculosis (TB) remains a major global health challenge, worsened by the rise of multidrug-resistant (MDR) strains and the limitations of current therapies. Despite advances, existing treatments often fail to fully eradicate the disease, highlighting the urgent need for safer, more effective drugs[1]. The growing prevalence of HIV further increases the risk of active TB. TB has now surpassed COVID-19 as the world's deadliest infectious disease since 2023[1,2]. This resurgence of TB is linked to weakened immunity from COVID-19 and healthcare disruptions, which led to a backlog of undiagnosed and untreated TB cases[1,2]. Current treatment regimens are long, complex, and often cause serious side effects. This study addresses these challenges by designing, synthesizing, and evaluating novel quinoline-benzoxaborole compounds as potential anti-TB agents.

The design of target compounds was guided by the structure–activity relationship (SAR) of bedaquiline, a recently approved drug for multidrug-resistant TB. The target compounds will be accessed using classical organic methods, involving multi-step reactions to construct the quinoline core and incorporate the benzoxaborole moiety under reflux conditions. The final products will be purified by recrystallization or chromatography, and their structures confirmed using various spectroscopic methods.

The synthesis of quinoline-benzoxaborole compounds is still ongoing, with successful preparation of five desirable intermediates necessary for the subsequent steps in the synthesis. The structures and purity of these intermediates were confirmed using spectroscopic techniques, including NMR, and IR. Molecular docking studies of proposed hybrids against *Mtb*-LeuRS and *Mtb*ATPase enzymes revealed favourable binding affinities and interactions. *In silico* ADME profiling, conducted using open-access tools, indicated that some of the compounds complied with Lipinski's Rule of Five. Further studies will include *in vitro* evaluation of anti-TB activity and assessment of toxicity and safety profiles.

While the preparation of the final compounds is underway, the preliminary in silico data of quinoline-benzoxaborole hybrids showed favourable binding affinity, drug-like properties, and potential for effective cellular uptake.

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Investigating the anti-inflammatory properties of *Harpephyllum caffrum* and its bioactive phytochemicals

Tatenda Machakaire, Fanie R. van Heerden, and Muvhango Rasalanavho

School of Agriculture and Science, Discipline of Chemistry, University of KwaZulu-Natal, Pietermaritzburg, South Africa, Email: 21700136@stu.ukzn.ac.za

Keywords: *Harpephyllum caffrum*, Inflammation, COX-2 inhibition, medicinal plants

Harpephyllum caffrum Bernh. ex Krauss, commonly known as the "wild plum", is a member of the Anacardiaceae family, the fourth largest tree family in Southern Africa [1]. Beyond its notable stature, *H. caffrum* is widely recognised for its diverse ethnomedicinal applications. Traditionally, various parts of the tree have been used to treat fractures, sprains, acne, and eczema [2,3]. These traditional uses have prompted scientific interest in its anti-inflammatory properties, particularly its potential to inhibit prostaglandin synthesis. Prostaglandins are essential mediators that play a central role in initiating the inflammatory response, and these mediators are produced via the metabolism of arachidonic acid by cyclooxygenase (COX) enzymes. Non-steroidal anti-inflammatory drugs (NSAIDs) alleviate pain by inhibiting this enzymatic pathway [4].

In this study, nine South African medicinal plants with documented ethnobotanical uses for pain and inflammation were collected, and lead-like extracts were prepared from different plant parts. The extracts (500 µg/mL extract solution) were screened using a colorimetric COX-2 enzyme inhibition assay (**Figure 1**). Among the assayed species, *H. caffrum* extracts demonstrated notable activity, with COX-2 inhibition levels of 45.6% and 41.6% observed in the stems and leaves, respectively, relative to the standard drug celecoxib. These results support the traditional use of *H. caffrum* in treating inflammatory conditions and highlight its potential as a source of novel anti-inflammatory compounds.

Consequently, the stem and leaf extracts were selected for further investigation, including bioassay-guided fractionation and compound isolation, to identify the active constituents responsible for COX-2 inhibition. This study contributes to the growing body of evidence affirming the pharmacological significance of South African medicinal plants. This research also highlights the importance of integrating ethnobotanical knowledge with contemporary drug discovery approaches.

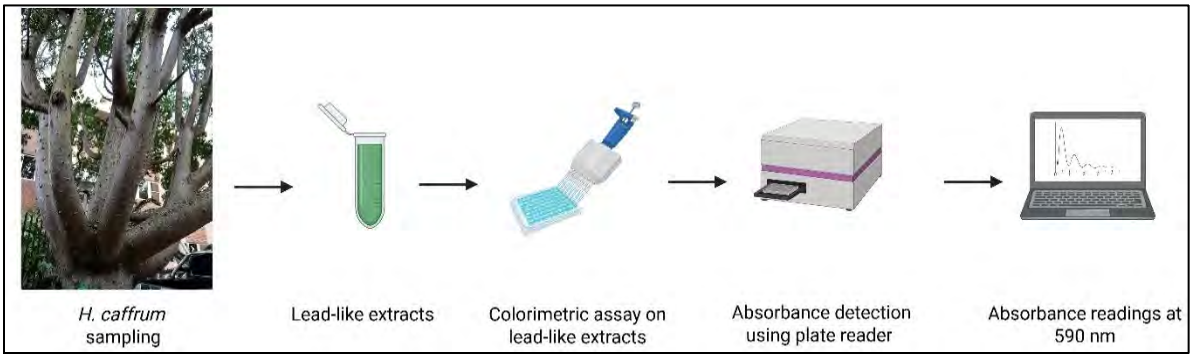

Figure 1. The process of identifying active lead-like extracts.

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Identification of natural antidiabetic agents in indigenous medicinal plants used to treat diabetes

Nkosinathi K. Ngcobo[a]*, Fanie R. van Heerden*[a]*, Muvhango Rasalanavho*[a] *and Theresa H. T. Coetzer*[b]

[a]School of Agriculture and Science, Discipline of Chemistry, University of KwaZulu-Natal, Pietermaritzburg, 3201 E-mail: *217025545@stu.ukzn.ac.za.* [b]School of Agriculture and Science, Discipline of Biochemistry, University of KwaZulu-Natal, Pietermaritzburg, 3201

Keywords: diabetes, lead-likeness, natural products

The rising prevalence of diabetes mellitus has increased the interest in new and safer treatments to manage the disease. The increasing mortality associated with diabetes highlights the urgency for effective and affordable natural antidiabetic agents [1]. In South Africa, diabetes is one of the leading causes of mortality. Traditional medicine has been used since ancient times and plays a significant role as an alternative medicine.

Many plants, including mango trees (*Mangifera indica*), marula trees (*Scelocarya birrea)*, rooibos tea (*Aspalathus linearis*), and honeybush tea (*Cyclopia subternata*), have been reported to exhibit antidiabetic activity [2,3]. Bioactive compounds isolated from these plants, for example, mangiferin, a compound present in mango leaves, show in vitro activity by inhibiting enzymes associated with diabetes and activity in in vivo experiments [4]. Suryawanshi et al. [4] reported that mangiferin shows comparable inhibitory activity to the standard antidiabetic drugs (sitagliptin, acarbose) against the diabetic enzyme targets DPP-4, α-glucosidase, and α-amylase. This study aimed to further investigate the inhibitory potential of these plants and to isolate the chemical constituents responsible for the antidiabetic activity. Small-scale lead-like extractions (on 300 mg of plant material) were prepared from the plants mentioned above. α-Glucosidase, α-amylase, and DPP-4 inhibitory assays were conducted on the extracts, which demonstrated significant inhibitory effects by some of the extracts. To identify the compounds in the extracts, profiling was performed using UPLC-MS. This presentation will report on the fractionation and isolation of active compounds using chromatographic techniques, with compound identification based on NMR and MS experiments.

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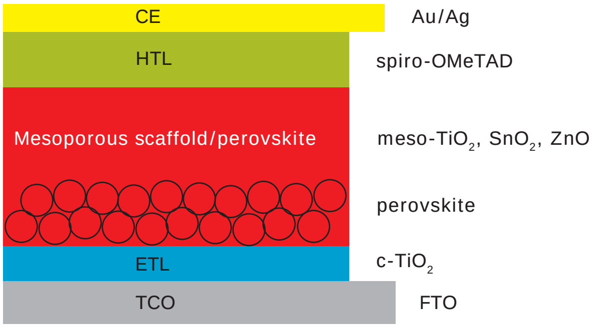

Name	Composition	Form	Prod. No.
Acetamidinium Iodide	$C_2H_7N_2I$	Powder	805971
Benzylammonium Iodide	$C_7H_{10}NI$	Powder	806196
i-Butylammonium Iodide	$C_4H_{12}NI$	Powder	805866
n-Butylammonium Iodide	$C_4H_{12}NI$	Powder	805874
t-Butylammonium Iodide	$C_4H_{12}NI$	Powder	806102
Diethylammonium Iodide	$C_4H_{12}NI$	Powder	806188
Dimethylammonium Iodide	C_2H_8NI	Powder	805831
Ethylammonium Iodide	C_2H_8NI	Powder	805823
Guanidinium Iodide	CH_6N_3I	Powder	806056
Formamidinium Iodide	CH_5N_2I	Powder	806048
Imidazolium Iodide	$C_3H_5N_2I$	Powder	805963
Methylammonium iodide	CH_6NI	Powder	793493
Methylammonium iodide	CH_6NI	Solution, 0.42 M in 2-propanol	808431
Methylammonium bromide	CH_6NBr	Powder	793507
Methylammonium bromide	CH_6NBr	Solution, 0.18 M in 2-propanol	808407
Phenylammonium Iodide	C_6H_8NI	Powder	805912
i-Propylammonium Iodide	$C_3H_{10}NI$	Powder	805882
n-Propylammonium Iodide	$C_3H_{10}NI$	Powder	805858

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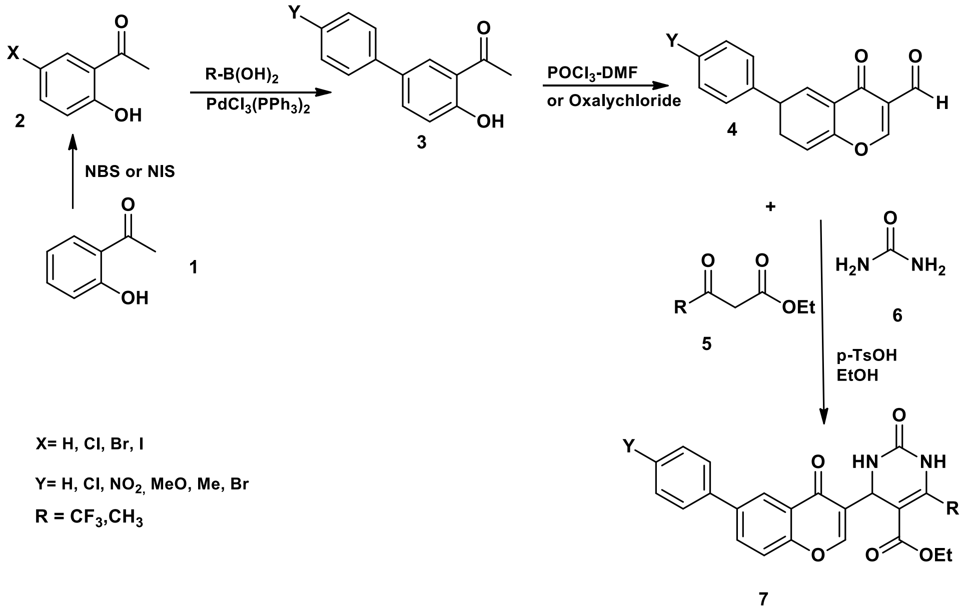
Synthesis of 6-substituted chromone-3-tetrahydropyrimidine based derivatives as potential anti-tuberculosis agents

Rolivhuwa Makotole R[a], Isaiah Ramaite [a], and Teunis Van Ree[a]

Department of Chemistry, University of Venda, Private Bag X 5050, South Africa, Thohoyandou, 0950
e-mail: Rolivhuwa.makotole@univen.ac.za

Keywords: *Acetophenone, Antitubercular drugs, Mycobacterium tuberculosis, Tuberculosis, Suzuki coupling, Vilsmeier reaction*

This study is aimed at the development of several precursors for the synthesis of biologically active 6-Substituted Chromone-3-Tetrahydropyrimidine derivates [1]. Starting with phenol to acetophenone or from acetophenone, several electrophilic aromatic substitution reactions, such as bromination and Suzuki coupling [2], reaction will be implemented to synthesize substituted acetophenone, which will be subsequent Vilsmeier reaction with oxalyl chloride/DMF and then transformed to substituted acetophenones, crucial intermediates for the synthesis of substituted acetophenone. All products will be characterized primarily by NMR, FTIR, PXRD and GC-MS spectroscopies [3].



Scheme 1: Synthesis of 6-subsituted chromone-3-tetrahydropyrimidines

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Design, green synthesis, and evaluation of coumarin-azabenzimidazole hybrids for anticancer therapy

Buhlebenkosi Zinyana[a], *Rosalyn Klein*[b]

First flr Rm 39 - 40 Chemistry & Pharmacy Bld, Cnr University & Ottery Road, Makhanda, 6139, E-mail: g19z5878@campus.ru.ac.za.

Keywords: Azabenzimidazole, Coumarin, Cyclin-dependent kinase (CDK) inhibition, Anticancer agents, Green chemistry, Sustainable drug synthesis

Uncontrolled cell division, resistance to apoptosis, and the emergence of multidrug resistance are the main causes of cancer, which continues to rank among the world's top causes of death. Even with major advancements in cancer treatment, there is still a pressing need for safer, more efficient, and more focused therapies. By creating, manufacturing, and characterizing a novel series of hybrid compounds that combine two pharmacologically preferred scaffolds—coumarin and azabenzimidazole—this study seeks to meet that demand. These scaffolds were chosen because they have complimentary anticancer qualities: coumarins can modify several cellular pathways and may be able to overcome drug resistance[1], while azabenzimidazoles have strong cyclin-dependent kinase (CDK) inhibitory activity[2].

To encourage sustainability and reduce the negative effects on the environment, green chemistry concepts were used throughout the synthetic process. The produced hybrids were structurally characterized by means of powder X-ray diffraction (PXRD), FTIR, and NMR. To verify molecular geometry and purity, single-crystal X-ray diffraction (SCXRD) was used where appropriate crystals could be produced. To determine the compounds' cytotoxicity and anticancer potential, in vitro bioassays were performed against certain cancer cell lines.

The goal of this research is to aid in the creation of next-generation anticancer drugs by incorporating dual-targeting mechanisms into a green synthetic framework. The results could provide a viable approach to stop tumor growth and combat multidrug resistance, which would advance the development of safer and more efficient cancer treatments.

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Design, synthesis, antimycobacterial evaluation, and computational studies of new quinazoline analogues

Safiyah Ghumran[a], *Baji Baba Shaik*[b] *and Parvesh Singh*[a]

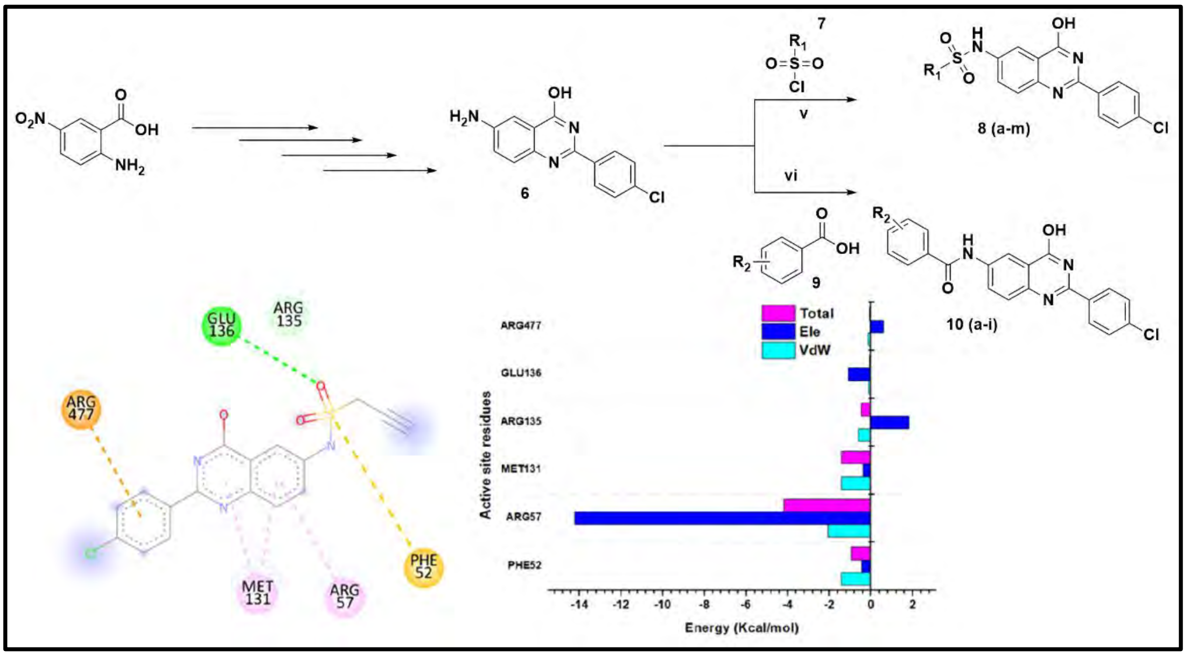
[a]Department of Chemistry, School of Agriculture & Science, Collage of Agriculture, Science, & Engineering, University of KwaZulu Natal, Private Bag X01, Scottsville, Durban, South Africa, E-mail: 214524354@stu.ukzn.ac.za. [b]Department of Pharmaceutical Chemistry, Discipline of Pharmaceutical Sciences, College of Health Sciences, University of KwaZulu-Natal, Westville Campus, Durban, South Africa

Keywords: Tuberculosis, H37Rv, DNA gyrase, Molecular dynamic simulation

Tuberculosis (TB) is an airborne disease that causes the death of tens of thousands of South Africans annually, despite being treatable. The co-infection of HIV and TB as well as the rise of drug-resistant strains of TB make treatment difficult. Thus, it is imperative to develop drugs that act against both multi drug-resistant and extremely drug-resistant TB (MDR and XDR).

A series of new quinazoline analogues (**8a-m** & **10a-i**) were designed, synthesized, and evaluated for their antitubercular activity, scheme shown below (**Scheme 1**). The final compounds were evaluated *in vitro* for their antitubercular and antimicrobial activity against a panel of pathogenic strains with Moxifloxacin, Rifampicin, Isoniazid, Ofloxacin and Levofloxacin as the standards. The compounds showing the highest inhibitory activity against *Mtb* H37Rv were compounds **8k** and **8m** with both having a minimum inhibitory concentration (MIC) of 3.9 µg/mL, the highest MIC thereafter came from compounds **8a**, **8l**, and **10h**.

Compounds **8a** and **8k** activity against MDR-TB and XDR-TB strains with MIC values of 7.81µg/mL and 15.62 µg/mL, respectively. When tested against select pathogenic fungi (*A. fumigatus*, *A. flavus*, *A. niger*) it was noted that compounds **8a**, **8b**, **8k** and **10h**, also exhibited significant activity with MIC values ranging from 3.9 to 15.62 µg/mL. In addition, DNA gyrase enzyme inhibition studies showed that **8l**, **8m**, and **10h** could inhibit at low micromolar levels (IC_{50} = 1.08–3.49 µM), indicating *Mtb* gyrase as the probable drug target. The docking and molecular dynamic simulations of select compounds indicated their binding modes and the crucial intermolecular interactions are similar to Ciprofloxacin, a known DNA gyrase inhibitor.



Investigations into the anti-cancer activity of 4'-substituted flavonols

Jenni Vrey[a,b], Nicky JD Verhoog[a], Amanda C Swart[a], Catherine H Kaschula[b]

[a]Department of Biochemistry, Stellenbosch University, Matieland 7600, South Africa. [b]Department of Chemistry and Polymer Sciences, Stellenbosch University, Matieland, 7600, South Africa. E-mail: jvrey@sun.ac.za.

Keywords: flavonols, phytomedicine, Hammett constant, androgen receptor, cancer

Cancer is a growing public health concern in South Africa, with10,065 new cases and 5528 deaths in 2020. Prostate cancer (PCa) is the most commonly diagnosed cancer among men, followed by lung cancer (LCa)[1]. Current therapies, such as androgen biosynthesis inhibitors and epidermal growth factor receptor inhibitors, are expensive and often have unwanted side effects, and can lead to the development of chemoresistance with long-term use. Flavonols are natural anticancer agents that show cytotoxicity towards cancer cells, and also modulate the androgen receptor (AR), a critical binding site for hormones responsible for PCa progression. The aim of this project is to synthesize two libraries of 4'-substituted flavonols (Figure 1) and to test them for cancer cell cytotoxicity against prostate and lung cancer cells, as well as their ability to modulate the activity of the AR. The proposed analogues were first investigated *in silico* for their potential binding interactions with the AR using Schrodinger's Maestro software. The promising analogues were then synthesized from the respective chalcone, which was oxidatively cyclized to the flavonol via the Algar-Flynn-Oyamada reaction in good yield. Investigation into the structure-activity effects found that ring deactivating substituents at the 4'-position of the flavonol enhanced cancer cell cytotoxicity in support of our previous findings[2]. We hypothesized that the acidity of the 3-OH group may be driving this effect, and this was investigated by measuring the respective pK_a's of the flavonols via spectrophotometric titration in aqueous solution. The findings of this work lay the foundation for developing a flavonol-based cancer therapeutic.

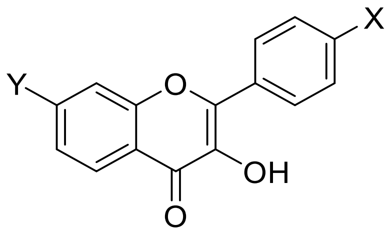


Figure 1: General structure of the flavonols of interest in this study. Y = H/OH, X = Br, F, I, Cl, Me, OMe, CH_3, SCH_3, SO_2CH_3, CF_3, OH.

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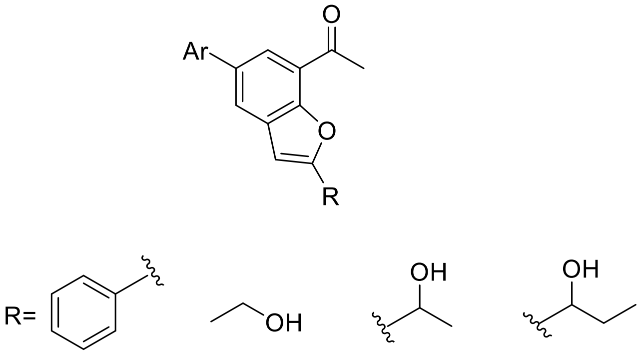
Design and synthesis of benzofuran derivatives as potential anti-tuberculosis agents

Mabula F[a], Nxumalo W[a]

[a]University of Limpopo, department of Chemistry, Private Bag x1106, Sovenga, 0727, Polokwane, South Africa, E-mail address: mafatefrans@gmail.com

Keywords: Benzofuran, Anti-Tuberculosis, Multidrug-resistant TB

Tuberculosis (TB) is a contagious disease mainly affecting the lungs but can spread to other organs. It is caused by bacteria in the *Mycobacterium tuberculosis* complex and spreads via airborne particles [1]. TB exists in latent and active forms, with the active form causing symptoms and transmission [2]. The rise of multidrug-resistant (MDR) and extensively drug-resistant (XDR) TB strains complicates treatment and highlights the need for new drugs. Benzofuran derivatives have shown diverse biological activities including antimicrobial and antiparasitic effects. Prado et al. identified benzofurobenzopyran compounds with selective anti-TB activity and minimal toxicity. TAM16, a benzofuran derivative, targets the Pks13 enzyme essential for mycobacterial cell wall synthesis and is effective against MDR-TB without cross-resistance This study aims to synthesize substituted benzofuran derivatives and evaluate their potential as anti-TB agents, expanding therapeutic options against resistant strains[3].



Ar= 3-FC$_6$H$_4$-; 4-MeOC$_6$H$_4$-; 4-CF$_3$C$_6$H$_4$-; C$_5$H$_3$S-

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Helichrysum caespititium and the Cape flora's medicinal heritage: Bioactive potential and ethnopharmacological applications for diabetes and disease management

Masixole Makhaba[a], Asavela Lupondo[a], Masande Yalo[a], Jonas Sagbo[a], Sylvester Omoruyi[b], and Ahmed A Hussein[a]

[a]Department of Chemistry, Cape Peninsula University of Technology, Symphony Way (off Robert Sobukwe Rd.), Bellville, 7535, South Africa, E-mail: makhabam@cput.ac.za. [b]Department of Anatomical Sciences, Wits University, Braamfontein Johannesburg, 2050, South Africa

Keywords: *Helichrysum*, phytochemistry, diabetes, Cape Flora

Diabetes mellitus, a chronic metabolic disorder characterized by hyperglycemia and inadequate insulin production [1], is projected to affect 853 million people by 2050 [2]. The Cape Floristic Region, home to over 9400 species of flowering plants, of which 69% are endemic [3], offers untapped potential for addressing this global crisis. This exceptional biodiversity is attributed to the unique climatic conditions (Mediterranean) and variety of habitat types, ranging from coastal dunes to montane shrublands [4]. Several species from the Asteraceae family like *Helichrysum caespititium* hold strong traditional and medicinal value, embodying the intersection of ecological wealth and traditional healing knowledge. Various plant parts have been used by cultural groups across South Africa to manage diabetes [5,6]. Despite growing interest in ethnopharmacology, critical gaps persist in the identification of bioactive metabolites responsible for such therapeutic effects. In this work, we investigated *H. caespititium*'s phytochemical profile and antidiabetic properties to validate its ethnobotanical use. Compounds were identified and characterized using nuclear magnetic resonance (NMR) spectroscopy and high-resolution electrospray ionization mass spectrometry (HRESIMS). Their bioactivities were assessed through various in vitro assays. Our results revealed interesting phytochemistry of the plant and promising bioactivities that validate its traditional use, though warranting further evaluation. In addition, this work highlights the importance of conserving *H. caespititium* and related species through sustainable harvesting, education and community involvement.

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Identification and isolation of metallo-β-lactamase inhibitory compounds from South African medicinal plants

Polette Refilwe Masiela[a,b,c], *Stephen Amoo*[a], *Vinesh Maharaj*[b], *Phanankosi Moyo*[b], *Samkelo Malgas*[c]
and Dashnie Naidoo-Maharaj[a,b]

[a]Agricultural Research Council-Vegetables, Industrial, and Medicinal Plants, Roodeplaat, 0039, South Africa, Email: MasielaR@arc.agric.za. [b]Biodiscovery Centre, Department of Chemistry, University of Pretoria, Hatfield, 0002, South Africa. [c]Department of Biochemistry, Genetics and Microbiology, University of Pretoria, Hatfield 0002, Gauteng, South Africa.

Keywords: Antimicrobial resistance, Metallo-β-lactamases, Serine-β-lactamases, Medicinal plants, Compounds

Antimicrobial resistance (AMR) of infectious disease-causing bacteria has emerged as one of the most critical global health threats, undermining the effectiveness of current antibiotic therapies. The metallo-β-lactamases (MBLs), produced by some bacteria, are of particular concern due to their ability to hydrolyse almost all β-lactam antibiotics, including the last-resort carbapenems. Despite extensive research, there remains a critical shortage of clinically approved MBL inhibitors, highlighting the urgent need for novel therapeutic strategies. Natural products, particularly medicinal plants, represent a promising yet underexplored source of bioactive compounds with potential MBL inhibitory activity. The South African medicinal plant, *Gunnera perpensa*, was evaluated *in vitro* for inhibitory activity primarily against a panel of clinically relevant MBLs, New Delhi Metallo-beta-lactamase-1 (NDM-1) and Verona Integron-encoded Metallo-beta-lactamase-1 (VIM-1); and secondarily against serine-β-lactamases (SBLs), TEM-116 (Temoniera-116) and OXA-10 (Oxacillinase-10); with captopril and avibactam sodium as positive controls. Dried leaf powder of *G. perpensa* was extracted using a dichloromethane-methanol solvent system (1:1, v/v). The resulting crude extract was fractionated by solid-phase extraction (SPE) using seven sequential solvent systems: methanol-water (5:95, Fraction 1), (20:80, Fraction 2), (40:60, Fraction 3), (60:40, Fraction 4), (80:20, Fraction 5), (100:0, Fraction 6), and acetonitrile-methanol (50:50, v/v; Fraction 7), targeting the compounds responsible for the bioactivity. Fraction 1 displayed IC_{50} values of 3.00 μg/mL against NDM-1, 5.00 μg/mL against VIM-1, and 0.90 μg/mL against both TEM-116 and OXA-10. Fraction 2 displayed IC_{50} values of 2.00 μg/mL against both NDM-1 and VIM-1, 0.80 μg/mL against TEM-116, and 0.90 μg/mL against OXA-10. Compared to the fractions, captopril showed IC_{50} values of 5.2 μg/mL against NDM-1 and 139.1 μg/mL against VIM-1, while avibactam sodium showed IC_{50} values of 1.1 μg/mL against TEM-116 and 12.4 μg/mL against OXA-10. Ultra-Performance Liquid Chromatography coupled with Quadrupole Time-of-Flight Mass Spectrometry (UPLC–QTOF–MS) analysis led to the tentative identification of orotic acid (Rt 0.9 min), linocaffein (Rt 4.36 min), skimmin (Rt 5.5 min), and agrimol B (Rt 13.8 min) in Fraction 1, with tricrozarin (Rt 1.9 min) additionally present in Fraction 2. Linocaffein and skimmin have been reported to have antimicrobial properties. Agrimol B has demonstrated antibacterial activity against plant pathogens, suggesting a defined antimicrobial potential. In contrast, tricrozarin has no documented evidence of antimicrobial activity. Molecular docking showed good binding affinity between the tentative compounds and the receptor. Isolation and structural characterisation of the compounds are in progress to identify the compounds responsible for the bioactivity. This will be followed by enzyme kinetics to determine inhibition constants and modes, and synergy testing with β-lactams to confirm restoration of antibiotic activity. These studies will advance the understanding of how plant-derived molecules inhibit beta-lactamases at the molecular level, providing mechanistic insights to guide rational design of next-generation inhibitors for combating antibiotic resistance.

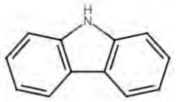
Synthesis and biological evaluation of carbazole-derivatives

Ian Mwanawene, Professor R. Klein

Department of chemistry, Rhodes University, 6139, Makhanda, South Africa, smigo2470@gmail.com

Keywords: carbazoles, fragment linking, metal-organic frameworks, porous coordination polymers, inclusion complexes, anti-cancer therapy

Carbazoles are natural alkaloids that exhibit interesting biological activity [1]. They are low molecular weight compounds and therefore have been widely used as templates in medicinal chemistry for drug designing and discovery [1-2]. Due to their low molecular weight, carbazoles tend to bind multiple targets [3]. However, their potency can be enhanced through fragment linking, fragment growing, and fragment merging [4-5]. Many studies have reviewed the carbazole potential in anti-cancer therapy and across other treatments. The approved carbazole-based derivatives used in anti-cancer therapy include ellipticine and others [6-7]. The proposed MSc study aims to offer a double knock in anti-cancer therapy through inclusion complexes, by taking advantage of carbazoles and metals. The objectives of this study include (**i**) synthesis of carbazole derivatives, (**ii**) linking of carbazole derivative(s) to metals towards metal-organic-frameworks (MOFs) synthesis, (**iii**) inclusion of other anti-cancer agents into carbazole-based MOFs, and (**iv**) biological evaluation of carbazole derivatives, carbazole-based MOFs and inclusion complexes.



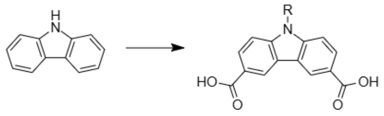


Figure 1: carbazole structural unit. **Figure 2**: Proposed synthetic scheme

Research has shown a high demand for carbazoles across various applications. Therefore, synthetic routes have been developed. Herein, carbazole derivatives are synthesized following the scheme below.Many studies have reviewed that linking carbazoles to metals may improve their stability, targeted delivery, bioavailability etc[8-10]. The proposed study will therefore take advantage of metals that possess therapeutic properties (Zn, Cu, Co) in order to provide a double knock in therapy.

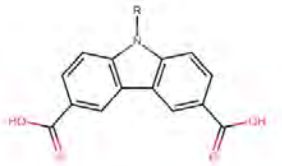


Figure 3: The general synthetic scheme and structure of MOFs. **Figure 4**: Carbazole dicarboxylate ligand

Carbazoles will be linked to metals, towards the synthesis of metal-organic-frameworks (MOFs). MOFs are crystalline porous coordination polymers. MOFs are used as drug delivery vehicles due to their crystalline-porous nature [8]. The proposed study will therefore take advantage of the porous nature of MOFs to include other anti-cancer agents. It is hypothesized that including other anti-cancer agents into carbazole-based MOFs, might yield better therapeutic properties.The carbazole dicarboxylate ligand has been used in the synthesis of cages. It has been proven to not disturb the formation of the cages due to its planarity and other properties [9]. Therefore, it can be inferred that other anti-cancer agents would be included in the carbazole-based MOFs smoothly.

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Targeted synthesis of fused heterocyclic-aromatic system from phenols with ortho-substituted 1,2,4-butanetriol

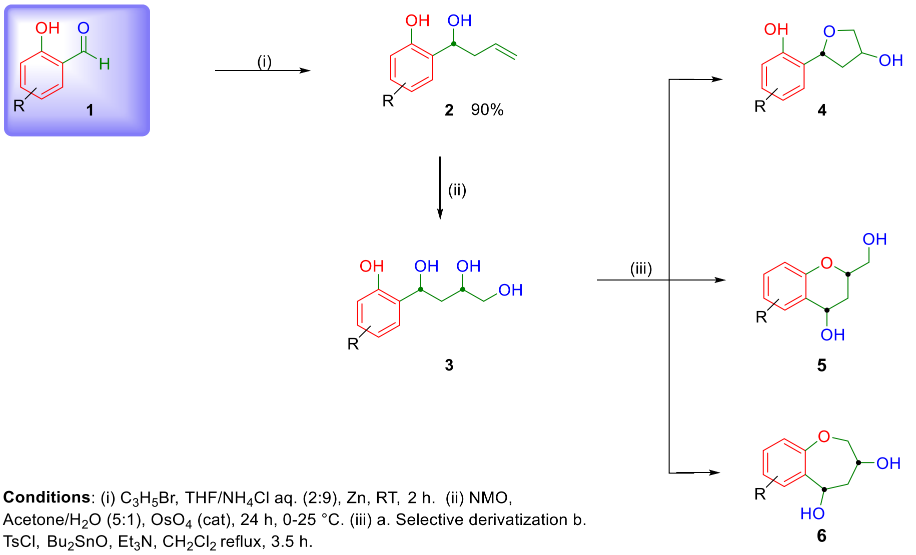
Thukwane T, *Nkambule CM*

Department of Chemistry, Tshwane University of Technology, Pretoria, 0001, South Africa, E-mail: ThukwaneT@tut.ac.za

Keywords: Derivatization, bicyclic compounds, cyclodehydration, benzopyran and benzoxepin.

Bicyclic compounds are found widely in natural and pharmaceutical products.[1] These include flavonoids, chromanoids, 2,3,4,5-Tetrahydro-1-benzoxepin, which have benzofuran, benzopyran and oxepine moieties, respectively. Compounds with these three moieties have been reported to exhibit a wide range of biological properties including antimicrobial, anticancer, antioxidant, and anti-inflammatory. [2]

Most medicinal chemists prefer to extract compound with complicated structures from plants, and that can be a tedious process and often with low yields of the desired product. The total isolation requires a lot of reagents and solvents. Often these compounds contain fused cyclic rings and many other functional groups; therefore, the total synthesis of these compounds with specific stereochemistry remains a huge challenge to chemists. Our hypothesis is that the three moieties of interest can be synthesized by selectively derivatizing hydroxyl groups of polyhydroxylated molecules followed by cyclodehydration as shown on scheme 1.[3]



Conditions: (i) C_3H_5Br, THF/NH_4Cl aq. (2:9), Zn, RT, 2 h. (ii) NMO, Acetone/H_2O (5:1), OsO_4 (cat), 24 h, 0-25 °C. (iii) a. Selective derivatization b. TsCl, Bu_2SnO, Et_3N, CH_2Cl_2 reflux, 3.5 h.

Scheme 1: Targeted synthesis of fused bicyclic rings using cyclodehydration and derivatizing techniques.

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QbD driven development of *Cissus quadrangularis* based ethosomal gel: In silico, in vitro, and in vivo evaluation

Abdullah S. Alshetaili

Department of Pharmaceutics, College of Pharmacy, Prince Sattam Bin Abdulaziz University, P.O. Box 173, Al-Kharj 11942, Saudi Arabia E-mail: a.alshetaili@psau.edu.sa.

Keywords: *In-silico*, ADMET analysis, Quality by design, *Cissus quadrangularis* extracts gel, Paw edama

The current study's goal was to create a gel formulation that contained *Cissus quadrangularis'* methanolic leaf extract and assess its anti-inflammatory properties using both in vitro and in vivo methods. The extract's anti-inflammatory properties were contrasted with those of beta-sitosterol, which was identified by its Protein Data Bank ID (PDB ID: 4IKI). Additionally, in the framework of medication development, absorption, distribution, metabolism, excretion, and toxicity (ADMET) profiling was carried out to evaluate the formulation's protection and therapeutic potential. The formulation parameters were optimized using a Quality by Design (QbD) methodology. Fourier-transform infrared spectroscopy (FTIR), zeta potential analysis, particle size determination, scanning electron microscopy (SEM), and entrapment assessment of efficacy were among the extensive physicochemical characterizations performed on the prepared gel. In order to guarantee formulation stability and usage, additional evaluations included measures of viscosity, spreadability, and pH. Nine extract suspensions were administered to in vitro tests to measure the drug concentration at 273 nm; the optimal formulation showed a 90% optimum drug release over a 10-hour period. Animal models were used in an in vivo anti-inflammatory investigation in which the volumes of paw edema in five different groups were monitored over the course of a day. The findings showed a notable decrease in inflammation, indicating that the modified Cissus quadrangularis gel formulation was therapeutically effective.

The molecular docking study confirms the anti-inflammatory therapeutic advantages, and the study's results might suggest that the gel formulation has more anti-inflammatory action than extract. ADMET analysis ensures both safety and therapeutic effects.

Design and synthesis of α-amino acid-based Ugi products

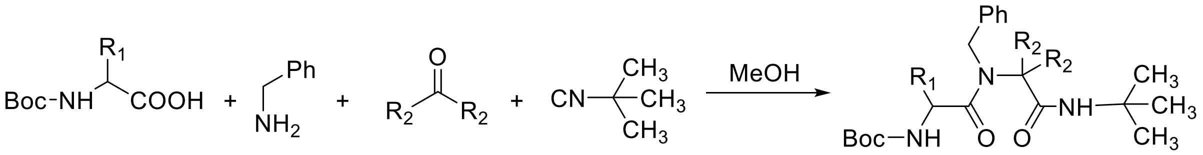
Alma Ramić, Sonia Hribar and Ines Primožič

Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, Croatia, E-mail: aramic@chem.pmf.hr.

Keywords: Ugi reaction, microwave-assisted synthesis, peptidomimetics, enzyme inhibitors

The Ugi multicomponent reaction is a valuable synthetic method that enables the assembly of peptide-like molecules in one step through the condensation of four building blocks: a carboxylic acid, an aldehyde (or ketone), an amine, and an isocyanide. The obtained peptide-like scaffolds often mimic natural products or bioactive peptides, thereby enhancing their probability of interacting with biological targets such as enzymes, receptors, or nucleic acids.[1] Some Ugi products have been investigated for their cholinesterase inhibitory activity, which is particularly important in the treatment of neurodegenerative diseases like Alzheimer's or Parkinson’s disease.[2, 3]

In this research, we have synthesized a small series of structurally related peptide-like compounds through the Ugi reaction by using different *N*-*tert*-butyloxycarbonyl (Boc) protected amino acids, formaldehyde or acetone, *tert*-butyl isocyanide and benzylamine. All compounds were synthesized by classical organic synthesis methods and by microwave-assisted organic synthesis. The course of the reactions was monitored by thin-layer chromatography, and the prepared compounds were purified by column chromatography. The structure of all prepared compounds was determined by 1D and 2D ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectroscopy and high-resolution mass spectrometry (HRMS). The inhibitory potential of all prepared compounds towards the enzyme butyrylcholinesterase (BChE, E.C. 3.1.1.8.) isolated from horse serum was determined by the Ellman method.[4]



R_1 - H; CH_2Ph; $CH_2C_8H_6N$

R_2 - H; CH_3

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Machine learning prediction of cholinesterase inhibition by 2-acylaminoacetamides

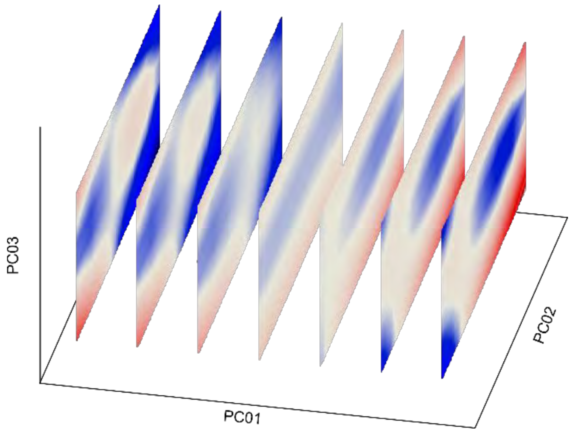
Ines Primožič and Tomica Hrenar

Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, Croatia, E-mail: ines.primozic@pmf.hr.

Keywords: Alzheimer's disease, cholinesterase inhibitors, 2-acylaminoacetamides, machine learning

Alzheimer's disease is a serious and worsening brain disorder that causes significant memory loss and thinking problems. One prominent idea about how Alzheimer's develops is the cholinergic hypothesis, which suggests that a decline in a brain chemical called acetylcholine contributes to these problems. Acetylcholine plays a crucial role in learning, memory, and attention, and its activity is regulated by acetylcholinesterase (AChE) and partially by butyrylcholinesterase (BChE). Because Alzheimer's damages brain cells and reduces acetylcholine production, cholinesterase inhibitors are used to increase acetylcholine levels in cholinergic synapses and help reduce symptoms. [1,2]

Predicting reversible inhibition from experimental data is a persistent challenge in modern science. In order to achieve this and use the prediction model for smart design, experimentally measured reversible inhibition data were regressed on the theoretically calculated potential energy surfaces (PES) of the new compounds investigated. Inhibition measurements of AChE and BChE were decomposed using principal component analysis, and principal components were used as regressors. As dependent variables, PES of the investigated compounds were used. In order to reduce them in dimensionality, tensor decomposition of PES sampled by *ab initio* molecular dynamics was performed. This provided the PES in reduced dimensions, which were used as dependent variables for modelling reversible inhibition. A machine learning protocol using multivariate linear regression [3] was employed to determine the best possible inhibition/PES regression model with a predicted R^2 value greater than 0.99. These results indicate that 2-acylaminoacetamides provide a promising starting point for designing and optimizing new cholinesterase inhibitors.



Best polynomial activity/PES regression model determined by machine learning.

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Concise total synthesis of (+)- and (-)-meranzin hydrate

Shrey Mokoena[a,b,c], *Derek Ndinteh*[b,c] *and Edwin Mmutlane*[a,b]

[a] Research Centre for Synthesis and Catalysis, Department of Chemical Sciences, University of Johannesburg, PO Box 524, Auckland Park 2006, Johannesburg, South Africa. [b] Centre for Natural Product Research (CNPR), Chemical Sciences Department, University of Johannesburg, Doornfontein 2028, Johannesburg, South Africa. [c] Drug Discovery and Smart Molecules Research Laboratory, Department of Chemical Sciences, University of Johannesburg, P.O. Box 17011, Doornfontein 2028, Johannesburg, South Africa, E-mail: edwinm@uj.ac.za.

Keywords: coumarin, meranzin hydrate, total synthesis

Ever since their isolation from Tonka beans by Vogel of Munich in 1820, Coumarin and its derivatives have been extensively studied and have been found to exhibit suitable biological activities, including anti-inflammatory, anti-cancer, and antimicrobial properties [1]. Among its derivatives, ulopterol **4** and meranzin hydrate **5** (isomers) exhibit a broad spectrum of pharmacological properties, rendering them effective antibacterial, antidepressant, anticoagulant, and anti-atherosclerotic agents [2]. From the consulted literature, ulopterol can be found on the leaves of *Toddalia asiatica* [3] and the fruit and roots of *Prangos uloptera* DC [4]. Meranzin hydrate has been isolated from *Muraya paniculata* and *Murraya exotica* [2,5]. Encouraged by meranzin hydrate's biological importance and intriguing structural features, we devised an enantioselective synthesis for meranzin hydrate, with the hope that the same methodology will be used to assemble, in a later stage, ulopterol (Figure **1**).

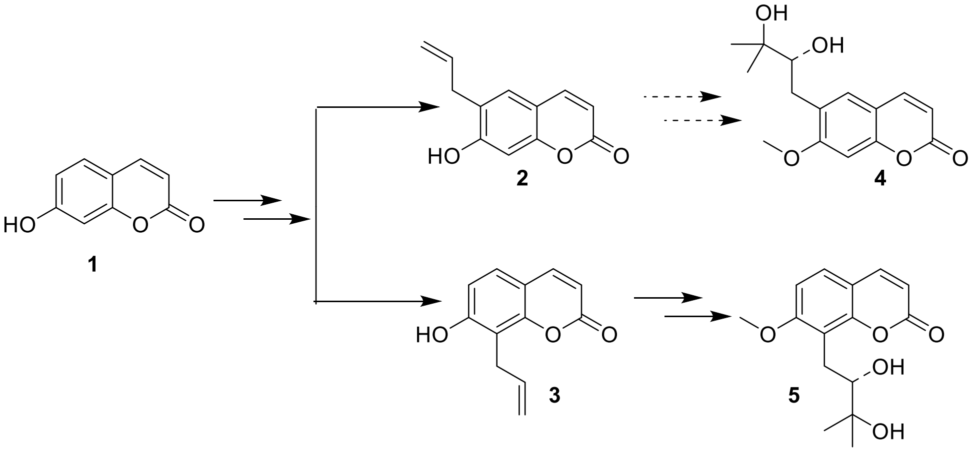

Figure 1. Synthesis of meranzin hydrate **5** and potential assembly of ulopterol **4.**

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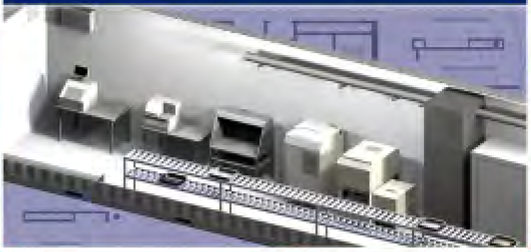

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JOHANNESBURG
T : +27 11 482 1060
wirsamjb@wirsam.com

CAPE TOWN
T : +27 21 386 9020
wirsamct@wirsam.com

DURBAN
T : +27 31 709 0199
wirsamdb@wirsam.com

PORT ELIZABETH
T : +27 41 365 2060
wirsampe@wirsam.com

VAAL TRIANGLE
T : +27 16 931 1731
wirsamvt@wirsam.com

Chemical investigation of the South African medicinal plant *Erythrina caffra* stem bark

Bienvenu Tsakem[a], *June Cheptoo Serem*[b], *Xavier Siwe Noundou*[a]

[a]Department of Pharmaceutical Sciences, School of Pharmacy, Sefako Makgatho Health Sciences University, South Africa, Email: 202432379@swave.smu.ac.za. [b]Department of Anatomy, School of Medicine, University of Pretoria, Pretoria, South Africa

Keywords: *Erythrina caffra*, spectroscopy, mass spectrometry, cytotoxicity, natural products

Erythrina caffra, a South African medicinal plant is traditionally used for various ailments. The plant remains underexplored with respect to its bioactive secondary metabolites.
This study aimed to isolate, characterize, identify, and evaluate the cytotoxicity of secondary metabolites from the stem bark of *E. caffra*.

The dried stem bark was extracted with CH_2Cl_2:MeOH (1:1) and partitioned into solvent fractions. While some chemical constituents were identified by LC-MS/MS using MassLynx, successive chromatographic techniques (silica gel and Sephadex LH-20) were employed for compound isolation. Structural elucidation was performed using FTIR, 1D and 2D NMR spectroscopy (^1H, ^{13}C, COSY, HSQC, HMBC) and HRESIMS. The cytotoxicity of the isolated compounds and fractions was assessed against human keratinocytes (HaCaT), melanocytes (NHEM-Ad), and hepatoma (HEPG2) using resazurin and crystal violet assays.

Compound isolation yielded 1 cerebroside, 3 flavonoids, and 5 phenolic acids. In addition, LC-MS^2 analysis allowed the tentative identification of twelve flavonoids and acyl feruloyl, supported by characteristic fragmentation patterns. Cytotoxicity assays showed that most isolated compounds were non-toxic to normal cell lines. However, two phenolic acids significantly reduced the viability of all three tested cell lines. Furthermore, both the crude extract and the ethyl acetate fraction markedly decreased cell viability in HaCaT and NHEM-Ad cells, suggesting the selective activity of certain constituents.

This work highlights the chemical diversity of *Erythrina caffra* stem bark and its potential as a source of bioactive natural products. Also, the study sets a foundation for future structure-activity relationship studies and drug discovery efforts.

Discrimination of isomers using hosts containing an imide functional group

Nyandano Netsianda and Eustina Batisai

Department of Chemistry, University of Venda, University Road, Thohoyandou, 0950, South Africa, E-mail: 20013614@mvula.univen.ac.za.

Keywords: cavity-based binding, host-guest complex, surface-based binding, picoline isomer

Host-guest chemistry is the branch of supramolecular chemistry concerned with the study of non-covalent interactions between a host compound and a guest [1]. The host is typically a crystalline material capable of accommodating guest species either through cavity-based inclusion or surface binding. Guests are compounds that are enclosed within or bound to the cavity or the binding sites of the host compound [2]. Host compounds can be organic or metal-organic and have numerous applications, one of the most prominent being liquid separation [3]. This process includes the separation of both isomeric and non-isomeric mixtures. This study focuses on isomeric mixture separation, which presents a significant challenge due to the structural similarities of isomers. Existing methods for separating isomers are often energy-intensive, costly, and complex [4].

This study investigates the ability of imide-functionalized host compounds to discriminate picoline isomers. We report the synthesis and characterization of two organic host molecules: 2-(carboxymethyl)-1,3-dioxoisoindoline-5-carboxylic acid (Host-1) and N-Phthaloylglycine (Host-2). These hosts were exposed to mixtures of picoline isomers, and the resulting host–guest complexes were analysed using single-crystal X-ray diffraction (SCXRD), powder X-ray diffraction (PXRD), gas chromatography (GC), and thermogravimetric analysis (TGA). Hirshfeld surface analysis was also performed to quantify the intermolecular interactions within the complexes. The findings from these techniques are discussed, with a focus on the host compounds' selectivity and preference for specific picoline isomers.

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Exploring the synthetic routes and phase stability of Bi-doped La_2Mo2O_9 oxide ion conductors

Emileo Naicker[1], *Caren Billing* [1,2], *David G. Billing*[1,2]

[1]*Molecular Science Institute, School of Chemistry,University of the Witwatersrand, Johannesburg, South Africa*
[2]*DSI-NRF Centre of Excellence in Strong Materials, University of the Witwatersrand, Private Bag X3, Johannesburg, South Africa.* emileo.naicker1@students.wits.ac.za

Fuel cells provide a way to convert chemical energy directly into electrical energy. In solid oxide fuels cells, the most commonly used electrolyte is yttrium-doped zirconia, but these cells need to operate above 800 °C to be sufficiently conducting [1]. The lanthanum molydate (LAMOX) family of materials also show great promise as electrolyte materials, with the high temperature $La_2Mo_2O_9$ β-phase having a higher oxide conductivity at lower temperatures. The phase change from the monoclinic phase to cubic β-phase occurs at 580 °C [2]. To stabilize the cubic phase at lower temperatures, substitution of the cationic and anionic sites is required. In this research, two different synthetic routes were explored with the focus being on bismuth as the substituent at the lanthanum site [3]. The two routes explored involved the normal solid-state route using intermediate grinding at 3 different heating steps (450 °C, 600 °C and 900 °C). The 2nd route involved the same heating steps however after each intermediate grinding, the sample was pressed into a pellet to promote integration and substitution of the bismuth ion and reduce impurities. X-ray diffraction results showed that both syntheses yielded very similar results, with 3% doped stabilizing the cubic phase of the LAMOX material however with minor impurities from both synthetic methods. This research is particularly important not only to investigate if bismuth will stabilize the cubic phase but also to investigate two different synthetic approaches as there are multiple approaches to synthesize the LAMOX materials.

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Er, W, Ta, and Ni-doped lanthanum molybdate: Enhancing β-phase stability and oxide transport

E. Porter[a], *C. Billing*[a] *and D. G. Billing*[a]

[a] Molecular Science Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Johannesburg 2000, South Africa. E-mail: 2380430@students.wits.ac.za

Keywords: Fast oxide ion conductor; SOEC; SOFC; VT-PXRD; VT-EIS

Lanthanum molybdate ($La_2Mo_2O_9$) is a well-known fast oxide ion conductor, offering significantly higher ionic conductivity compared to yttria stabilized zirconia (YSZ) at similar temperatures.[1] This makes it a promising candidate for use as an electrolyte in solid oxide fuel cells and electrolyzer cells (SOFCs/SOECs). However, it has not been commercial adopted due to a structural phase change at 580℃ from the α to β phase and chemical instability in oxidizing environments. Despite this, the potential gain in device efficiency due to greater ionic conductivity continues to drive research interest in lanthanum molybdate and its derivatives.[2]

This study investigates lanthanum molybdate derivatives, obtained via doping the parent material with various cations (Er^{3+}, W^{6+}, Ta^{5+}, Ni^{2+}) in a range of combinations and concentrations. These cations were chosen for their similar ionic radii to the cations sites they would occupy and their variation in valency. Structural analysis via powder X-ray diffraction (PXRD) and Rietveld refinement confirmed that the doped materials crystallize in the cubic ($P2_13$) β-phase at room temperature. The β-phase is the higher conducting phase of lanthanum molybdate and is typically only stable above 580℃ in the parent material. The thermal expansion of the materials was also determined via variable temperature PXRD by tracking lattice constants as a function of temperature. The electrochemical performance of the materials was measured using electrochemical impedance spectroscopy as a function of temperature as well.

The results demonstrate that doping stabilizes the β-phase at room temperature, reduces the coefficient of thermal expansion and increases ionic conductivity in the intermediate temperature range compared to that of the parent material.

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Optimizing the cubic phase stability and ionic transportation in Co-doped Lamox-based electrolytes

Caitlyn Habana[a], *Caren Billing*[a] *and Dave Billing*[a]

[a]Molecular Science Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa, E-mail: 2430032@students.wits.ac.za.

Keywords: fuel cells, cationic doping, solid state, oxide ion conductivity

Energy production and consumption remain a pressing issue in the present day due to a multitude of factors, including rapid population growth, urbanization, and industrial activity [1]. This leads to resource shortages, price fluctuations, and inequitable access [2]. Fossil fuels remain the primary source of electrical energy generation, but this results in the production of harmful air pollutants, including carbon dioxide [3]. This work focuses on solid oxide fuel cells (SOFCs), which are high-temperature (600 - 1000°C) fuel cells used to convert chemical energy into electrical energy, thereby minimizing the release of harmful air pollutants. SOFCs have a solid electrolyte used for ionic conduction and electronic insulation. The high operating temperatures, however, introduce challenges such as thermal expansion, material degradation, and increased costs [4]. Thus, the design of solid electrolyte materials that can operate at lower temperatures (400-600 °C) is crucial.

Lamox ($La_2Mo_2O_9$) exists in a monoclinic crystalline phase (α-$La_2Mo_2O_9$) with a $P2_1$ space group up to 580 °C and exhibits relatively low ionic conductivity (**Figure a**). Upon further heating, the system undergoes a phase change into a high-symmetry cubic phase (β-$La_2Mo_2O_9$) with a $P2_13$ space group, which exhibits high ionic conductivities (**Figure b**) [5]. To stabilize β-$La_2Mo_2O_9$ to room temperature and improve its ionic conductivity, cationic doping is introduced. In the Lamox structure, the dopants are expected to occupy the lanthanum (La^{3+}) and molybdenum (Mo^{6+}) sites. The choice of dopants is based on similarities in ionic radius and oxidation states between the dopants and the metal within the crystal lattice. This work looks at incorporating Er^{3+} (1.062 Å) at the La^{3+} (1.216 Å) site to stabilize the cubic phase and Al^{3+} (0.535 Å) at the Mo^{6+} (0.59 Å) site to increase oxide vacancies and reduce the extent of reduction of Mo^{6+} to Mo^{4+} when in a reducing atmosphere, thus improving the ionic conductivity when compared to undoped Lamox.

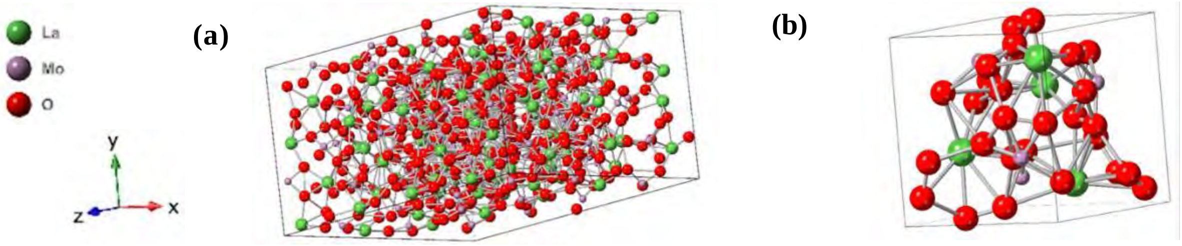

Figure: (**a**) The α-$La_2Mo_2O_9$ (monoclinic) crystal structure with a $P2_13$ space group and (**b**) the β-$La_2Mo_2O_9$ (cubic) with a $P2_1$ space group

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Machine learning and DFT-driven design of spinel $Zn_xMn_{1-x}Co_2O_4$ as bifunctional electrocatalysts for rechargeable zinc-air batteries

Naledi Khati, *Aderemi B. Haruna, Desalegn N. Gemechu, Thapelo P. Mofokeng, Kenneth I. Ozoemena*

[a]Molecular Science Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Johannesburg, 2050, South Africa, E-mail: 2490730@students.wits.ac.za.

Keywords: Density Functional Theory

The global transition toward sustainable energy systems demands high-performance, cost-effective, and environmentally friendly energy storage technologies. Rechargeable zinc–air batteries (RZABs) stand out due to their high theoretical energy density, safety, and abundance of raw materials [1]. However, their commercialization remains limited by sluggish oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) kinetics. The development of low-cost, bifunctional electrocatalysts that are both efficient and durable under alkaline conditions remains a critical challenge [2]. This study seeks to address these limitations through the rational design of bifunctional electrocatalysts based on spinel $\mathrm{Zn_xMn_{1-x}Co_2O_4}$ (x = 0.2, 0.4, 0.6, 0.8). We integrate experimental synthesis, density functional theory (DFT), and machine learning (ML) to accelerate the electrocatalysts optimization. The hydrothermally synthesized electrocatalysts catalysts are physico-chemically and electrochemically characterized, while DFT simulations are used to extract electronic descriptors such as adsorption energies of oxygen intermediates $(\mathrm{O^*, OH^*, OOH^*})$, d-band centre, surface energies and density of states (DOS). These features informed supervised ML models trained to predict and rank catalytic performance across compositions for ORR/OER activities. The central hypothesis is that partial substitution of Mn with Zn will induce electronic structure modifications such as oxygen vacancy generation and d-band centre tuning which will enhance the material's ORR and OER activity. Experimental data is compared with ML predictions to validate the model's robustness and guide the selection of optimal electrocatalyst compositions. This study aims to uncover property relationships that govern ORR/OER bifunctionality, reduce reliance on precious metals, and minimize trial-and-error experiments in electrocatalysts discoveries. Ultimately, this work demonstrates a data-driven pathway for faster design of materials for sustainable energy storage.

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Computational drug design of novel compounds targeting poly [ADP-Ribose] polymerase 1 (PARP-1) for breast cancer treatment

Charmy Twala[a], *Penny Govender*[a], *Emphraim Marondedze*[a] *and Krishna Govender*[a]

[a]Department of Chemical Sciences, University of Johannesburg, Doornfontein Campus, P.O. Box 17011, Doornfontein, 2028, South Africa

Keywords: Breast cancer, Poly [ADP-Ribose] polymerase 1 (PARP-1), Artificial Intelligence-driven Drug Design (AIDD), Synthetic lethality, PARP inhibition

Breast cancer is one of the leading causes of cancer-related deaths globally and has overtaken cervical cancer as the most common cancer among Indian women [1–3]. Poly [ADP-ribose] polymerase-1 (PARP-1), an enzyme involved in DNA repair, is a validated target for cancers with BRCA1/2 mutations [4]. Although FDA-approved PARP inhibitors such as Olaparib have shown efficacy, their clinical use is limited by cardiotoxicity due to off-target effects [5]. This study applied Artificial Intelligence-driven Drug Design (AIDD) within a synthetic lethality framework to develop novel PARP-1 inhibitors with improved safety and efficacy. A multi-step computational workflow-comprising molecular docking, compound enumeration, density functional theory (DFT), molecular dynamics (MD) simulations, MM/GBSA binding free energy analysis, and high-throughput pharmacokinetics (HTPK) - was used to optimize compound properties. The newly generated compounds were assessed for drug-likeness, absorption, and toxicity, enabling early identification of promising candidates. Key physicochemical properties were refined to enhance solubility and bioavailability without compromising target specificity. Comparative docking studies revealed that several leads had more favourable interaction profiles with the PARP-1 active site than existing drugs. DFT-based analyses, including HOMO-LUMO gap studies, confirmed strong electronic stability and reactivity. The integration of these approaches allowed for the rational prioritization of candidates with both therapeutic potential and minimized off-target risks. The top leads showed higher binding affinity and stability compared to Olaparib, with favourable electronic characteristics and pharmacokinetic profiles. Notably, redocking and cardiotoxicity screening confirmed reduced off-target interactions with the hERG1 channel. These findings suggest that the newly designed PARP-1 inhibitors offer a safer and more effective therapeutic option for BRCA-mutated breast cancer.

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[2] D.M. Parkin, F. Bray, J. Ferlay and A. Jemal. Cancer in Africa. Cancer Epidemiol. Biomark. Prev. 23 (2014): 953–966.
[3] K. Kaarthigeyan. Cervical cancer in India and HPV vaccination. Indian J. Med. Paediatr. Oncol. 33 (2012): 7–12.
[4] J.A. Ledermann, Y. Drew and R.S. Kristeleit. Homologous recombination deficiency and ovarian cancer. Eur. J. Cancer 60 (2016): 49–58.
[5] A.N. Tutt et al. Adjuvant olaparib for patients with BRCA1- or BRCA2-mutated breast cancer. N. Engl. J. Med. 384 (2021): 2394–2405.

PDT activity studies for AAAB, ABAB, AABB, ABBB and BBBB Sn(IV) tetrapiperidinylphenylporphyrins

Pertunia R. Macigane, John Mack and Tebello Nyokong

Institute for Nanotechnology Innovation, Rhodes University, Makhanda 6140, South Africa, E-mail: j.mack@ru.ac.za

Keywords: tetraarlyporphyrins, photodynamic therapy, ligand docking, TD-DFT, photophysics

There is considerable interest in Sn(IV) tetraarylporphyrins due to their heavy atom effect that increases the singlet oxygen quantum yield and their *trans*-axial ligation, which eliminates aggregation effects [1]. These properties make them more favourable for use in photodynamic therapy (PDT), which is a non-invasive procedure that uses light and porphyrinoids to cause tumour cell death [2-3]. The rationale behind this work is to perform theoretical calculations to evaluate the effect of structural modification of porphyrinoids on their spectroscopic and optical properties. The effects of the transition from mono- to tetrapiperidinylphenyl substitution of the tetraphenylporphyrin structure in an AAAB, ABAB, AABB, ABBB, BBBB series (A=phenyl, B=piperidinylphenyl), metalation with an Sn(IV) ion and quaternisation of the piperidinyl phenyl nitrogen atom were evaluated. The BBBB complex is predicted to have the most red shifted Q band, potentially making it more favourable for PDT as it lies deeper within the phototherapeutic window (620−850 nm). The results of *in vitro* PDT activity studies.

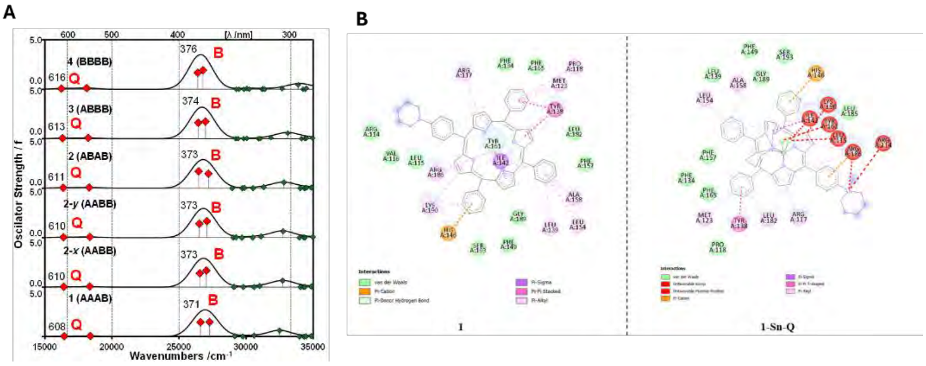

Figure 1. (A) TD-DFT simulated spectra. (B) HSA binding interaction with AAAB

Molecular docking was conducted to predict the binding affinities of the porphyrins to the human serum albumin (HSA) transport protein. It was concluded that AAAB has the highest binding energy, and, therefore, is more likely to be transported to the tumour cells. The porphyrinoids are predicted to have exceptional ADMET properties and to be non-carcinogenic. The predicted pharmacological properties of the porphyrins all violate Lipinski's rule of five. They likely could not be used as orally active drugs but could be administered as intravenous injections for PDT in a similar manner to Photofrin®. During *in vitro* PDT activity studies against MDA-MB-231 cells, the ABAB and AABB porphyrins were found to have the most favourable IC_{50} values, possibly due to aggregation issues that were encountered with the ABBB and BBBB porphyrins.

[1] Babu, B.; Mack, J.; Nyokong, T. *Dalton Transactions* 2023, **52**, 5000-5018.
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[3] Babu, B.; Amuhaya, E.; Oluwole, D.; Prinsloo, E.; Mack, J.; Nyokong, T. *MedChemComm* 2019, **10**, 41-48.


SCIEX
X500R QTOF

In silico molecular modelling of paclitaxel and its derivatives targeting microtubules in breast cancer

Sharna Moonsamy[a], *Krishna Govender*[b], *Brian Flepisi*[c] *and Marissa Balmith*[a]

[a]Department of Pharmacology, Faculty of Health Sciences, School of Medicine, University of Pretoria, Pretoria, South Africa E-mail: u20416386@tuks.co.za. [b]Department of Chemical Sciences, University of Johannesburg, Johannesburg, South Africa~~.~~ [C]Department of Pharmacy and Pharmacology, University of the Witwatersrand, Johannesburg, South Africa

Keywords: breast cancer, paclitaxel, microtubules, molecular docking, molecular dynamics simulations

Most breast cancer mortalities are due to metastasis, where microtubules are a key regulator of migration and invasion. Paclitaxel, a tubulin-targeting chemotherapeutic, remains effective but is limited by drug resistance and significant toxicity. This study aimed to determine the binding affinity, binding free energy and molecular dynamics (MD) simulations of paclitaxel, and its *in silico* derivatives in breast cancer cells.

The ChEMBL database was screened for small molecules inhibitors with ≥85% structural similarity to paclitaxel. Four tubulin isoforms (5LXT, 4I4T, 6SES and 1TUB) were selected for molecular docking using Glide, Maestro. Thereafter, molecular mechanics with generalised born surface area (MM/GBSA) binding free energy calculations were conducted. The best performing isoform was taken further for docking followed by MM/GBSA. A 100-nanosecond MD simulation was performed using Desmond.

A total of 323 compounds were obtained from ChEMBL. The target, PDB: 6SES, was the best performing isoform based on MM/GBSA calculations and was used for subsequent docking. Among the screened compounds, 7-epi-paclitaxel and 2’-Acetyltaxol demonstrated intermediate and weak binding, with docking scores of –0.014 kcal/mol and –5.220 kcal/mol, and MM/GBSA binding free energies of –64.53 kcal/mol and –60.70 kcal/mol, respectively. Ligand root mean square deviation (RMSD) of 7-epi paclitaxel has higher fluctuations as the RMSD is around 4.5Å while 2’-Acetyltaxol does not exceed 3Å.

The findings showed moderate and weak stability of 7-epi paclitaxel and 2’-acetyltaxol in the active site, respectively. Additionally, these findings support the use of 7-epi paclitaxel as an improved therapeutic candidate. These findings prompt the investigation of the effects of 7-epi paclitaxel and 2’-Acetyltaxol on microtubules in breast cancer cells and their potential as improved therapeutic candidates.

Perturbations of the hydroxyl group of phenol by chlorine substituents

Potlaki F Tsekj

Department of Chemical & Physical Sciences, Walter Sisulu University Nelson Mandela Drive, Mthatha 5099, South Africa.

Keywords: Substituent perturbation, fundamental frequency, fluorobenzene

In this work we use experimental and calculated fundamental vibrations stretching frequencies and calculated torsional energies for the side chain hydroxyl group to investigate its response to mono-chlorine substitutions on the phenol ring. It appears that the electronic charge density resulting from substituent perturbations on the ring is transmitted from the chlorine **p-type** atomic orbitals through the π* anti-bonding atomic orbitals of the ring carbons to the **p-type** atomic orbitals of the heteroatom to elicit an electronic perturbation response by the side chain hydroxyl group. As it turns out, the magnitudes and directions of change, due to substituent perturbations, for both vibrational and the torsional energies for the side chain hydroxyl group appear to be closely correlated. The perturbation resulting from chlorine substitution on the aromatic ring reveals that these two internal motions; vibration and rotation for the hydroxyl moiety are constants of motion for the side chain group as a system[1]. We interpret this behaviour as evidence of conservation of the angular momentum for the side chain hydroxyl group.

A perturbation response by the hydroxyl group of phenol to chlorine substitution on the ring manifested through both the torsional barriers and fundamental vibrational frequencies.

Torsional barrier potentials for the hydroxyl group of phenol

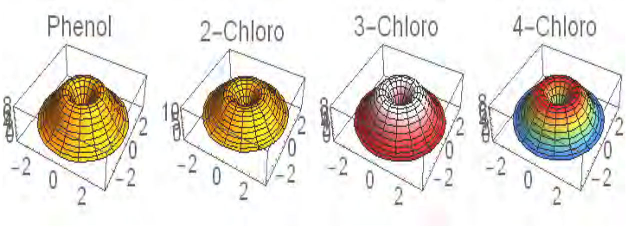


Figure. The torsional energy distribution profiles for phenol and its mono chlorine substituted derivatives; the 2-chloro derivative indicates the highest torsional energy barrier.

[1] Ira N. Lavine, Quantum Chemistry, 7th Ed.

INDEX

ID	Surname	Name	Venue	Day	Time
P35	Adegbenga	Idowu	Flower Hall		
P98	Adeleke	Adesola	Flower Hall		
O105	Adesanya	Funmilola	WSS3	Wednesday	11h50-12h10
P21	Adeyemi	Jerry	Flower Hall		
O119	Akerele	Oluwatoyi	WSS3	Thursday	10h30-10h50
O43	Akinola	Akinshola	WSS2	Monday	14h55-15h15
O48	Akwi	Faith	WSS3	Monday	10h50-11h10
P141	Alshetaili	Abdullah	Flower Hall		
P34	Arotiba	Omotayo	Flower Hall		
O13	Azov	Vladimir	WSS4	Thursday	14h00-14h55
P88	Baabua	Ketshepile	Flower Hall		
P53	Babaee	Saeideh	Flower Hall		
O8	Baker	Priscilla	WSS4	Monday	14h00-14h55
P68	Bamisaye	Abayomi	Flower Hall		
O103	Banda	Kabelo	WSS3	Wednesday	11h10-11h30
O16	Barran	Perdita	WSS3	Friday	10h30-11h25
O80	Bepete	George	WSS2	Tuesday	11h30-11h50
P1	Berkenbosch	Neale	Flower Hall		
O59	Billing	Dave	WSS4	Monday	11h30-11h50
P116	Biyela	Nosipho	Flower Hall		
O4	Blackie	Margaret	WSS2	Thursday	8h50-10h00
O10	Brits	Martin	WSS2	Tuesday	14h00-14h55
O1	Bryant-Friedrich	Amanda	WSS2	Monday	8h50-10h00
O74	Bucibo	Malesole	WSS2	Tuesday	15h15-15h35
O70	Bvumbi	Mpelegeng	WSS2	Tuesday	11h10-11h30
O55	Byamungu	Galilee	WSS3	Monday	16h20-16h40
O56	Carroll	Robert	WSS4	Monday	10h30-10h52
P129	Chaka	Delight	Flower Hall		
O60	Chatterjee	Nabanita	WSS4	Monday	11h50-12h10
P26	Chernet	Helen	Flower Hall		
O137	Chetty	Shaeen	WSS5	Thursday	11h10-11h30
P100	Chota	Grace	Flower Hall		
P126	Damona	Eldon	Flower Hall		
P54	Dansoa	Frank	Flower Hall		
O114	Danso-Boateng	Eric	WSS2	Thursday	11h30-11h50
O125	de Langa	Jurgens	WSS3	Thursday	15h15-15h35
P93	Dembaremba	Tendai	Flower Hall		
P16	Dlangalala	Celiwe	Flower Hall		
O110	Dube	Sifelani	WSS4	Wednesday	11h50-12h10
P22	Dube	Sifelani	Flower Hall		
O66	El-Hendway	Morad	WSS5	Monday	16h00-16h20
O138	Esiefa	Winifred	WSS5	Thursday	11h30-11h50
P77	Fapojuwo	Dele	Flower Hall		
O145	Feleni	Gwibaka	WSS4	Friday	11h25-11h45
O6	Fine	David	SHB5	Sunday	14h00-16h00
O38	George	Midhun	WSS2	Monday	10h30-10h50
P134	Ghumran	Safiyah	Flower Hall		
O128	Ginqi	Abongile	WSS4	Thursday	10h50-11h10
P149	Habana	Caitlyn	Flower Hall		

ID	Surname	Name	Venue	Day	Time
O88	Habib	Nejat	WSS4	Tuesday	10h50-11h10
O147	Haruna	Aredemi	WSS4	Friday	12h05-12h25
P27	Hechter	Ernst	Flower Hall		
O12	Heeren	Ron	WSS2	Thursday	14h00-14h55
P95	Hlatshwayo	Zamangwane	Flower Hall		
P38	Hlongwane	Mokgadi	Flower Hall		
O18	Hunter	Roger	Great Hall	Sunday	17h00-17h50
O63	Iwuoha	Benneth	WSS4	Monday	16h00-16h20
O28	Jayaraman	N.	WSS4	Tuesday	14h00-14h30
O73	Kannigadu	Christina	WSS2	Tuesday	14h55-15h15
P23	Kannigadu	Christina	Flower Hall		
O29	Keinan	Ehud	WSS2	Thursday	16h30-17h00
O108	Kgabi	Dipuo	WSS4	Wednesday	11h10-11h30
O21	Khan	Malik Dilshad	WSS2	Monday	12h10-12h45
P150	Khati	Naledi	Flower Hall		
P50	Khoza	Karabo	Flower Hall		
P91	Khoza	Keneilwe	Flower Hall		
P46	Khuboni	Sbusiso	Flower Hall		
O76	Khumalo	Mathew	WSS2	Tuesday	16h20-16h40
O5	Klampfl	Christian	WSS2	Friday	8h50-10h00
O112	Kontile	Lelethu	WSS2	Thursday	10h50-11h10
O86	Kotze	Izak	WSS3	Tuesday	16h20-16h40
P127	Kotze	Tyla	Flower Hall		
P55	Kunene	Neliswa	Flower Hall		
O77	Lai	Wing-Fu	WSS3	Tuesday	10h30-10h50
P83	Lale	Lesedi	Flower Hall		
o53	Langa	Carol	WSS3	Monday	15h15-15h35
O52	Langmi	Henrietta	WSS3	Monday	14h55-15h15
O57	Lau	Tracy	WSS4	Monday	10h50-11h10
O146	Lebechi	Agustus	WSS4	Friday	11h45-12h05
O45	Lebepe	Thabang	WSS2	Monday	16h00-16h20
P58	Ledibane	Mmabatho	Flower Hall		
P73	Ledwabaa	Mahlatse	Flower Hall		
P7	Lehabe	Karabo	Flower Hall		
P9	Lekalakala	Vanessah	Flower Hall		
O120	Lemmerer	Andreas	WSS3	Thursday	10h50-11h10
P110	Lepedia	Tsholofelo	Flower Hall		
P25	Leso	Masejeng	Flower Hall		
O49	Lokole	Pathy	WSS3	Monday	11h10-11h30
O134	Mabatamela	Lebogang	WSS4	Thursday	15h35-15h55
P136	Mabula	F	Flower Hall		
O144	Machakaire	Tatenda	WSS3	Friday	11h45-12h05
P130	Machakaire	Tatenda	Flower Hall		
P152	Macigane	Pertunia	Flower Hall		
O50	Mack	John	WSS3	Monday	11h30-11h50
P123	Madasi	Sinoxolo	Flower Hall		
O24	Madikizela	Lawrence	WSS2	Thursday	12h10-12h45
P47	Madingwane	Augustine	Flower Hall		
O106	Madonsela	Nomaswazi	WSS4	Wednesday	10h30-10h50
P84	Mafentile	K	Flower Hall		
P79	Magagula	Lindokuhle	Flower Hall		

ID	Surname	Name	Venue	Day	Time
O46	Magqira	Bavuyile	WSS2	Monday	16h20-16h40
P103	Magunda	T.K	Flower Hall		
P74	Magwaza	Temlandvo	Flower Hall		
P89	Mahlaka	Ndiphiwe	Flower Hall		
P37	Mahlambi	Precious	Flower Hall		
O39	Mahlangu	Maki	WSS2	Monday	10h50-11h10
P43	Makasi	Beatice	Flower Hall		
O22	Makatini	Maya	WSS2	Friday	12h25-13h00
P87	Makgaka	Thato	Flower Hall		
P137	Makhaba	Masixole	Flower Hall		
P90	Makhumisane	Phathutshedzo	Flower Hall		
P132	Makotole	Rolivhuwa	Flower Hall		
O80	Makume	Boitumelo	WSS3	Tuesday	11h30-11h50
P106	Malebadi	K.A	Flower Hall		
O133	Maluleke	Blesant	WSS4	Thursday	15h15-15h35
P117	Malusela	T	Flower Hall		
o140	Mametja	Sense	WSS2	Friday	11h25-11h45
O23	Mammino	Liliana	WSS2	Thursday	12h45-13h20
O47	Manye	Remofilwe	WSS3	Monday	10h30-10h51
O41	Mapetla	Sabetha	WSS2	Monday	11h30-11h50
P11	Maphoru	Mabuatsela	Flower Hall		
O90	Maseko	Paula	WSS4	Tuesday	11h30-11h50
O117	Masemola	Lethabo	WSS2	Thursday	15h15-15h35
O132	Mashaba	Chakes	WSS4	Thursday	14h55-15h15
P138	Masiela	Polette	Flower Hall		
O69	Masivuye	Mahleba	WSS2	Tuesday	10h50-11h10
P122	Mathenjwa	Mandisa	Flower Hall		
P12	Mathole	R	Flower Hall		
P109	Maubane-Nkadimene	Manoko	Flower Hall		
P20	Mautla	Mpho	Flower Hall		
O99	May	Aviwe	WSS2	Wednesday	11h30-11h50
P120	Mayoli	Simamkele	Flower Hall		
P31	Mbande	Zukiswa	Flower Hall		
P39	Mbatha	Thandeka	Flower Hall		
O95	Mbayo	Vitalis	WSS4	Tuesday	16h20-16h40
P78	Mbongo	Relebohile	Flower Hall		
P97	Mbumbulwana	Luzuko	Flower Hall		
P57	Mbuyi	Joyce	Flower Hall		
P14	McAdam	Ross	Flower Hall		
P108	Medupe	Thato	Flower Hall		
P49	Miya	Motlalepule	Flower Hall		
P29	Mlozana	Yibanathi	Flower Hall		
O92	Mnyakeni	Simon	WSS4	Tuesday	14h55-15h15
P28	Mnyandu	Hopewell	Flower Hall		
P33	Mofokeng	T	Flower Hall		
O143	Mojela	Nare	WSS3	Friday	11h25-11h45
O27	Mokaya	Robert	WSS3	Monday	14h00-14h55
P144	Mokoena	Shrey	Flower Hall		
P96	Molapo	Tshegofatso	Flower Hall		
O118	Molaudzi	Nesieni	WSS2	Thursday	15h35-15h55

ID	Surname	Name	Venue	Day	Time
O111	Molebatsi	Mothusi	WSS2	Thursday	10h30-10h50
P80	Molefe	M	Flower Hall		
P94	Molefi	Botle	Flower Hall		
O113	Moloi	Sello	WSS2	Thursday	11h10-11h30
P105	Moloto	K.B	Flower Hall		
O115	Momanyi	Naom	WSS2	Thursday	11h50-12h10
P44	Monama	Salphy	Flower Hall		
O96	Moodley	Thrineshen	WSS2	Wednesday	10h30-10h50
O107	Moodley	Cresten	WSS4	Wednesday	10h50-11h10
P153	Moonsamy	Sharna	Flower Hall		
P32	Morake	Lebohang	Flower Hall		
O141	Moreki	Mbali	WSS2	Friday	11h45-12h05
P107	Moremi	Harold	Flower Hall		
O40	Moswane	Ramasehle	WSS2	Monday	11h10-11h30
P24	Mouton	Michaela	Flower Hall		
O124	Moyo	Cyprian	WSS3	Thursday	14h55-15h15
P102	Moyo	Pamela	Flower Hall		
P71	Mphephu	Rotondwa	Flower Hall		
P119	Mqilingwa	Phumzile	Flower Hall		
O93	Mtetwa	Bridget	WSS4	Tuesday	15h15-15h35
P42	Mthembu	Ntombifuthi	Flower Hall		
P52	Mthombeni	Harmony	Flower Hall		
O131	Mubiayi	Pierre	WSS4	Thursday	11h50-12h10
P121	Mudanabula	Ritshidze	Flower Hall		
P62	Mudau	Rendani	Flower Hall		
O116	Mugari	Mufaro	WSS2	Thursday	14h55-15h15
P48	Mukaba	Jean-Luc	Flower Hall		
O44	Mukanya	Jonathan	WSS2	Monday	15h15-15h35
P92	Mukwevho	Maano	Flower Hall		
P63	Murangi	Musingadi	Flower Hall		
P139	Mwanawene	Ian	Flower Hall		
O72	Myburgh	Lisa	WSS2	Tuesday	11h50-12h10
P147	Naicker	Emileo	Flower Hall		
O142	Ndlovu	Samantha	WSS2	Friday	12h05-12h25
P10	Ndlovu	Fathima	Flower Hall		
P146	Netsianda	Nyandano	Flower Hall		
P65	Netsianda	Nyandano	Flower Hall		
O42	Nevondo	Vhodaho	WSS2	Monday	11h50-12h10
O62	Ng'andu	Clever	WSS4	Monday	15h15-15h35
P131	Ngcobo	Nkosinathi	Flower Hall		
P30	Ngoepe	Nkgaetsi	Flower Hall		
P112	Ngubane	Ntombenhle	Flower Hall		
P76	Ngubane	Buyane	Flower Hall		
P104	Ngwenya	Simphiwe	Flower Hall		
P81	Ngwenya	Asanda	Flower Hall		
O75	Nhlapho	Samukelisiwe	WSS2	Tuesday	16h00-16h20
O135	Nkambule	Comfort	WSS5	Thursday	10h30-10h50
P56	Nkomana	Wendy	Flower Hall		
P67	Nkosi	Nonhlanhla	Flower Hall		
O54	Nkwachukwu	Oluchi	WSS3	Monday	16h00-16h20
P36	Nnaji	Nnaemeka	Flower Hall		

ID	Surname	Name	Venue	Day	Time
O11	Nocanda	Xolani	WSS3	Tuesday	14h00-14h55
P99	Nogqala	Simnikiwe	Flower Hall		
O26	Nolan	Michael	WSS4	Tuesday	12h10-12h45
O102	Nompetsheni	Indiphile	WSS3	Wednesday	10h50-11h10
O89	Nowakowska	Monika	WSS4	Tuesday	11h10-11h30
O109	Nsibande	Sifiso	WSS4	Wednesday	11h30-11h50
P59	Nthapo	Boitumelo	Flower Hall		
P69	Nthehang	Tsholofelo	Flower Hall		
O15	Nyamori	Vincent	WSS2	Friday	10h30-11h25
P18	Nyembe	Siyabonga	Flower Hall		
O127	Ogunlaja	Adeniyi	WSS4	Thursday	10h30-10h50
O122	Ojo	Babatope	WSS3	Thursday	11h30-11h50
P111	Okafor	Nnamdi	Flower Hall		
O68	Okechikwu	Viola	WSS2	Tuesday	10h30-10h50
P61	Oladipo	Segun	Flower Hall		
O94	Olalekan	Temitope	WSS4	Tuesday	16h00-16h20
O19	Ozoemena	Kenneth	Great Hall	Sunday	17h50-18h40
O126	Pant	Divya	WSS3	Thursday	15h35-15h55
O78	Patel	Mahmood	WSS3	Tuesday	10h50-11h10
P6	Phasha	Mildred	Flower Hall		
P45	Pholosi	Agnes	Flower Hall		
P124	Phophi	Hlamulo	Flower Hall		
O136	Pilcher	Lynne	WSS5	Thursday	10h50-11h10
P148	Porter	Ethan	Flower Hall		
O14	Potgieter	Marietjie	WSS5	Thursday	14h00-14h55
P143	Primožič	Ines	Flower Hall		
O64	Quesne	Matthew	WSS5	Monday	14h55-15h15
P115	Ragedi	Mashaole	Flower Hall		
P3	Ramaite	Isaiah	Flower Hall		
P118	Ramba	L	Flower Hall		
P64	Rambevha	Lesedi	Flower Hall		
P142	Ramić	Alma	Flower Hall		
O101	Ramonyai	Masego	WSS3	Wednesday	10h30-10h50
O79	Rampersadh	Pradish	WSS3	Tuesday	11h10-11h30
P13	Ratsoma	Nomthandazo	Flower Hall		
O58	Recchia	Daniella	WSS4	Monday	11h10-11h30
P8	Rohman	Tanya	Flower Hall		
O20	Rohwer	Egmont	WSS2	Wednesday	12h30-13h20
O139	Rollnick	Marissa	WSS5	Thursday	11h50-12h10
O51	Roman	Stacey	WSS3	Monday	11h50-12h10
O67	Ruwizhi	Ngonidzas	WSS5	Monday	16h20-16h40
O98	Rylands	Marwaan	WSS2	Wednesday	11h10-11h30
P51	Saban	Waheed	Flower Hall		
O123	Salajee	Atiyyah	WSS3	Thursday	11h50-12h10
P75	Samsodien	M	Flower Hall		
O3	Scholes	Greg	WSS2	Wednesday	8h50-10h00
P66	Sekaleli	Bafokeng	Flower Hall		
O130	Seleka	Wilson	WSS4	Thursday	11h30-11h50
O81	Sewpersad	Nikisha	WSS3	Tuesday	11h50-12h10
O83	Shnier	Adam	WSS3	Tuesday	14h55-15h15
P85	Sibambo	Thabiso	Flower Hall		

ID	Surname	Name	Venue	Day	Time
P4	Sibiya	Witness	Flower Hall		
P41	Simbanegavi	Prisca	Flower Hall		
P128	Sishi	Aphiwe	Flower Hall		
P2	Smuts	Thea	Flower Hall		
P60	Snyman	Brithney	Flower Hall		
O129	Sookai	Sheldon	WSS4	Thursday	11h10-11h30
O7	Stark	Annegret	WSS2	Monday	14h00-14h55
O91	Swarts	Andrew	WSS4	Tuesday	11h50-12h10
P72	Tauyakhale	Kaisano	Flower Hall		
P40	Thethwayo	Sinenhlahla	Flower Hall		
P140	Thukwane	T	Flower Hall		
P114	Tlhapi	Bafedile	Flower Hall		
O17	Tromp	Moniek	WSS4	Friday	10h30-11h25
P145	Tsakem	Bienvenu	Flower Hall		
P154	Tseki	Potlaki	Flower Hall		
O65	Tshaka	Menezi	WSS5	Monday	15h15-15h35
P113	Tshiluka	Ndivhuwo	Flower Hall		
P17	Tshiololi	Matodzi	Flower Hall		
P70	Tsoeu	Seiso	Flower Hall		
P86	Tumeli	Ts’epo	Flower Hall		
P151	Twala	Charmy	Flower Hall		
O104	Ukachi	Racheal	WSS3	Wednesday	11h30-11h50
P82	van Dyk	Rika	Flower Hall		
O82	van Eeden	Nestor	WSS3	Tuesday	12h10-12h30
O9	van Sittert	Cornie	WSS5	Monday	14h00-14h55
O87	van Zyl	Werner	WSS4	Tuesday	10h30-10h50
O85	Venter	Andrew	WSS3	Tuesday	16h00-16h20
P135	Very	Jenni	Flower Hall		
O61	Vitshima	Anati	WSS4	Monday	14h55-15h15
O121	Vorgers	Jarryd	WSS3	Thursday	11h10-11h30
O84	Walmsley	Ryan	WSS3	Tuesday	15h15-15h35
O2	Wasserscheid	Peter	WSS2	Tuesday	8h50-10h00
P101	Wazirit	Ibrahim	Flower Hall		
O25	Weigand	Jan	WSS2	Tuesday	12h10-12h45
O97	Wright	Sarah	WSS2	Wednesday	10h50-11h10
P15	Xolo	Luthando	Flower Hall		
P19	Yizengaw	Mulusew	Flower Hall		
O100	Zimuwandeyi	Memory	WSS2	Wednesday	11h50-12h10
P133	Zinyana	Buhlebenkosi	Flower Hall		
P5	Zondo	Sandisiwe	Flower Hall		
P125	Zulu	Delisile	Flower Hall		

The South African Council for Natural Scientific Professions (SACNASP) is the registration and regulatory body for natural science professionals in South Africa. SACNASP was established in terms of the Natural Scientific Professions Act (27 of 2003) (the NSP Act) as amended by the Science and Technology Laws Amendment Act (7 of 2014). The Council is mandated as the Accounting Authority to implement the provisions of the NSP Act, under the oversight of the Minister of Science and Innovation.

SACNASP's 5 years strategic objectives are to:

- To increase the number of registered natural science professionals, ensure greater retention, and enhance the efficiency of the registration process.
- To ensure high professional and ethical standards for natural science professionals.
- To promote the professional development and transformation of the natural scientific professions through lifelong learning programmes.
- To enhance and promote the contribution of the natural scientific professions through science communication and engagement.
- To foster strategic partnerships and collaborations in the advancement of the natural scientific professions.

CMP Programme

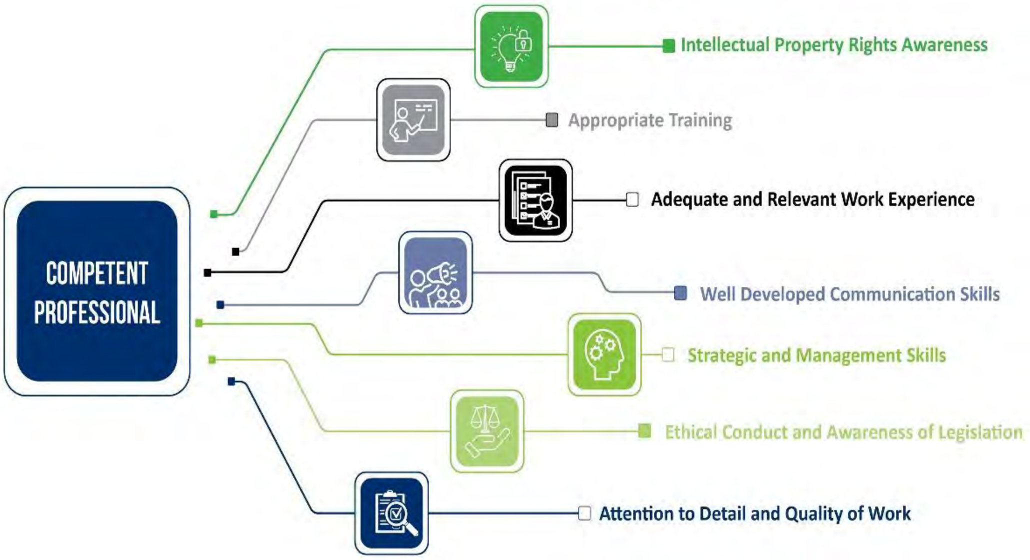
The Candidate Mentoring Phase (CMP) programme was implemented in FY2020/21

The programme is aimed at building a pipeline for the next generation of skilled natural science professionals in South Africa.

Ensure transformation in the percentage representation of natural science graduates from designated groups viz. women and marginalised groups.

SACNASP, in collaboration with the VA's, is assisting graduates to be ready for work by providing them with the skills relevant to their field of practice.

Continuing Professional Development (CPD)



Use the portal to update personal details and to download certificates:

https://portal.sacnasp.org.za/login

Follow links for Advisory note and the Practice note

https://www.sacnasp.org.za/advisory-notes

https://www.sacnasp.org.za/practice-notes

SACNASP'S Achievements

We are proud to share two significant achievements:

20,000 scientists have successfully registered with SACNASP this is a testament to the growing strength and unity of our scientific community.

The new SACNASP Board has been appointed, bringing fresh leadership and vision to guide us into the future.